

=> d his ful

(FILE 'HOME' ENTERED AT 14:09:07 ON 25 JUL 2005)

FILE 'CAPLUS' ENTERED AT 14:09:13 ON 25 JUL 2005

E US2004-816128/APPS

L1 67 SEA ABB=ON PLU=ON BRANDVOLD?/AU  
L2 0 SEA ABB=ON PLU=ON LEWIS?/AU AND L1  
L3 1218 SEA ABB=ON PLU=ON KING L?/AU  
L4 1693 SEA ABB=ON PLU=ON LEWIS G?/AU  
L5 0 SEA ABB=ON PLU=ON L3 AND L4  
L6 0 SEA ABB=ON PLU=ON L1 AND L4  
L7 350 SEA ABB=ON PLU=ON BREWER L?/AU  
L8 1 SEA ABB=ON PLU=ON L7 AND (L4 OR L3 OR L1)  
D SCA TI  
E HYDROPEROXIDES/CT  
E E3+ALL  
L9 1430 SEA ABB=ON PLU=ON HYDROPEROXIDES+PFT,NT/CT(L) PREP+ALL/RL

FILE 'REGISTRY' ENTERED AT 14:12:04 ON 25 JUL 2005

L10 6069 SEA ABB=ON PLU=ON "HYDROPEROXIDE"  
L11 STR  
L12 50 SEA SSS SAM L11  
L13 11585 SEA SSS FUL L11

FILE 'CAPLUS' ENTERED AT 14:13:19 ON 25 JUL 2005

L14 5326 SEA ABB=ON PLU=ON L13(L) PREP+ALL/RL  
L15 5810 SEA ABB=ON PLU=ON L9 OR L14

FILE 'REGISTRY' ENTERED AT 14:14:14 ON 25 JUL 2005

FILE 'CAPLUS' ENTERED AT 14:14:17 ON 25 JUL 2005

FILE 'REGISTRY' ENTERED AT 14:16:07 ON 25 JUL 2005

L\*\*\* DEL TRA L15 1- RN : 50608 TERMS

FILE 'REGISTRY' ENTERED AT 14:16:07 ON 25 JUL 2005

FILE 'CAPLUS' ENTERED AT 14:16:28 ON 25 JUL 2005

L16 1225 SEA ABB=ON PLU=ON L15 AND PY>1998  
L17 1716 SEA ABB=ON PLU=ON L15 AND PY>1995  
L18 4094 SEA ABB=ON PLU=ON L15 NOT L17

FILE 'REGISTRY' ENTERED AT 14:17:03 ON 25 JUL 2005

FILE 'CAPLUS' ENTERED AT 14:17:06 ON 25 JUL 2005

L19 TRA L17 1- RN : 23938 TERMS

FILE 'REGISTRY' ENTERED AT 14:17:27 ON 25 JUL 2005

L20 23938 SEA ABB=ON PLU=ON L19

FILE 'CAPLUS' ENTERED AT 14:23:58 ON 25 JUL 2005

L21 TRA L18 1- RN : 33989 TERMS

FILE 'REGISTRY' ENTERED AT 14:24:49 ON 25 JUL 2005

L22 33987 SEA ABB=ON PLU=ON L21  
L23 54744 SEA ABB=ON PLU=ON L20 OR L22  
L24 986 SEA ABB=ON PLU=ON L23 AND (MN OR CO OR CR OR V OR MO OR FE

OR CU OR NI)/ELS  
E OXYGEN/CN  
L25 1 SEA ABB=ON PLU=ON OXYGEN/CN  
SEL RN  
L26 400 SEA ABB=ON PLU=ON L25 OR 7782-44-7/CRN  
  
FILE 'CAPLUS' ENTERED AT 14:28:03 ON 25 JUL 2005  
L27 180563 SEA ABB=ON PLU=ON L24 (L) (CAT/RL OR ?CATAL?)  
L28 53387 SEA ABB=ON PLU=ON L26 (L) RACT+ALL/RL  
L29 523 SEA ABB=ON PLU=ON L15 AND L27  
L30 47 SEA ABB=ON PLU=ON L29 AND L28

FILE 'REGISTRY' ENTERED AT 14:29:08 ON 25 JUL 2005  
L\*\*\* DEL STR

FILE 'CASREACT' ENTERED AT 14:29:48 ON 25 JUL 2005  
L31 STR  
L32 2 SEA SSS SAM L31 ( 10 REACTIONS)  
L33 30 SEA SSS FUL L31 ( 248 REACTIONS)

FILE 'STNGUIDE' ENTERED AT 14:34:01 ON 25 JUL 2005

FILE HOME

FILE CAPLUS

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FILE COVERS 1907 - 25 Jul 2005 VOL 143 ISS 5  
FILE LAST UPDATED: 24 Jul 2005 (20050724/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 JUL 2005 HIGHEST RN 856767-39-0  
DICTIONARY FILE UPDATES: 24 JUL 2005 HIGHEST RN 856767-39-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

#### FILE CASREACT

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FILE CONTENT:1840 - 24 Jul 2005 VOL 143 ISS 4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

\*\*\*\*\*  
\*  
\* CASREACT now has more than 9.2 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

#### FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jul 22, 2005 (20050722/UP).

=> dup rem l33 l30

FILE 'CASREACT' ENTERED AT 14:34:15 ON 25 JUL 2005  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CAPLUS' ENTERED AT 14:34:15 ON 25 JUL 2005  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)  
PROCESSING COMPLETED FOR L33  
PROCESSING COMPLETED FOR L30  
L34           76 DUP REM L33 L30 (1 DUPLICATE REMOVED)  
              ANSWERS '1-30' FROM FILE CASREACT  
              ANSWERS '31-76' FROM FILE CAPLUS

=&gt; d que stat l33

L31 STR

RRT RRT PRO G1 8 Mn @9 Co @10 Cr @11

C~H O~O C~O~OH  
 1 2 6 7 3 4 5

V @12 Mo @13 Fe @14 Cu @15 Ni @16

VAR G1=9/10/11/12/13/14/15/16

NODE ATTRIBUTES:

NSPEC IS RC AT 1  
 NSPEC IS RC AT 3  
 NSPEC IS RC AT 9  
 NSPEC IS RC AT 10  
 NSPEC IS RC AT 11  
 NSPEC IS RC AT 12  
 NSPEC IS RC AT 13  
 NSPEC IS RC AT 14  
 NSPEC IS RC AT 15  
 NSPEC IS RC AT 16  
 CONNECT IS E1 RC AT 6  
 CONNECT IS E1 RC AT 7  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

## \*\*\*\*MAPPINGS\*\*\*\*

NOD SYM ROL NOD SYM ROL  
 1 C RRT 3 C PRO  
 3 C PRO 1 C RRT  
 L33 30 SEA FILE=CASREACT SSS FUL L31 ( 248 REACTIONS)

100.0% DONE 2043 VERIFIED 248 HIT RXNS 30 DOCS  
 SEARCH TIME: 00.00.01

=&gt; d que stat l30

L9 1430 SEA FILE=CAPLUS ABB=ON PLU=ON HYDROPEROXIDES+PFT,NT/CT(L) PREP  
 +ALL/RL  
 L11 STR

C~O~OH  
 1 2 3

NODE ATTRIBUTES:

NSPEC IS RC AT 1  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

## STEREO ATTRIBUTES: NONE

L13 11585 SEA FILE=REGISTRY SSS FUL L11  
L14 5326 SEA FILE=CAPLUS ABB=ON PLU=ON L13(L)PREP+ALL/RL  
L15 5810 SEA FILE=CAPLUS ABB=ON PLU=ON L9 OR L14  
L17 1716 SEA FILE=CAPLUS ABB=ON PLU=ON L15 AND PY>1995  
L18 4094 SEA FILE=CAPLUS ABB=ON PLU=ON L15 NOT L17  
L19 TRANSFER PLU=ON L17 1- RN : 23938 TERMS  
L20 23938 SEA FILE=REGISTRY ABB=ON PLU=ON L19  
L21 TRANSFER PLU=ON L18 1- RN : 33989 TERMS  
L22 33987 SEA FILE=REGISTRY ABB=ON PLU=ON L21  
L23 54744 SEA FILE=REGISTRY ABB=ON PLU=ON L20 OR L22  
L24 986 SEA FILE=REGISTRY ABB=ON PLU=ON L23 AND (MN OR CO OR CR OR V  
OR MO OR FE OR CU OR NI)/ELS  
L25 1 SEA FILE=REGISTRY ABB=ON PLU=ON OXYGEN/CN  
L26 400 SEA FILE=REGISTRY ABB=ON PLU=ON L25 OR 7782-44-7/CRN  
L27 180563 SEA FILE=CAPLUS ABB=ON PLU=ON L24(L)(CAT/RL OR ?CATAL?)  
L28 53387 SEA FILE=CAPLUS ABB=ON PLU=ON L26(L)RACT+ALL/RL  
L29 523 SEA FILE=CAPLUS ABB=ON PLU=ON L15 AND L27  
L30 47 SEA FILE=CAPLUS ABB=ON PLU=ON L29 AND L28

=&gt; d l34 ibib abs crd 1-30

L34 ANSWER 1 OF 76 CASREACT COPYRIGHT 2005 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 126:343150 CASREACT

TITLE: Preparative Oxidation of Organic Compounds in  
Microemulsions with Singlet Oxygen Generated  
Chemically by the Sodium Molybdate/Hydrogen Peroxide  
System

AUTHOR(S): Aubry, Jean-Marie; Bouttemy, Sabine

CORPORATE SOURCE: Faculte de Pharmacie de Lille, CNRS URA 351, Lille,  
F-59006, Fr.

SOURCE: Journal of the American Chemical Society (1997),  
119(23), 5286-5294

CODEN: JACSAT; ISSN: 0002-7863

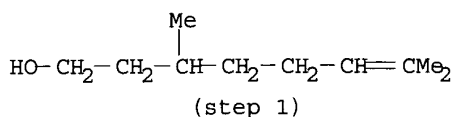
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

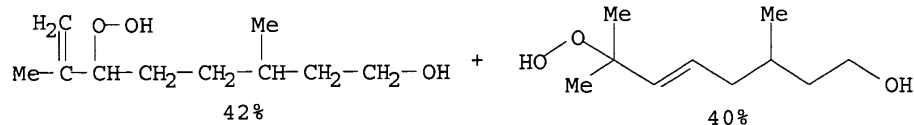
LANGUAGE: English

AB A reverse (water in oil) microemulsion has been designed to oxidize hydrophobic organic substrates with singlet oxygen ( $^1O_2$ ,  $^1\Delta_g$ ) generated by the disproportionation of hydrogen peroxide catalyzed by molybdate ions. The microemulsion was prepared by mixing methylene chloride, SDS, 1-butanol, and aqueous molybdate. Steady-state and flash photolysis studies have shown that in such media singlet oxygen exhibits a kinetic behavior similar to that under homogeneous conditions ( $\tau\Delta \approx 42$   $\mu$ s). Various typical organic substrates have been oxidized on a preparative scale with this chemical generated singlet oxygen, and the expected oxidation products have been isolated in high yields.

RX(7) OF 10



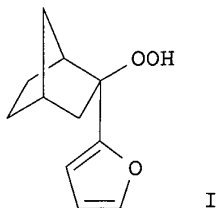
1. R:7631-95-0,  
Dodecyl Na sulfate,  
BuOH, Water,  
CH<sub>2</sub>Cl<sub>2</sub>
2. H<sub>2</sub>O<sub>2</sub>



NOTE: SINGLET OXYGEN PREPD. IN SITU BY PEROXIDE INTERACTION WITH MICROEMULSION

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

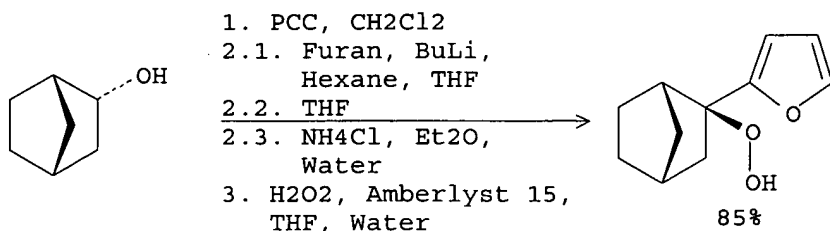
L34 ANSWER 2 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 141:190557 CASREACT  
 TITLE: Synthesis of a renewable hydroperoxide from  
 (+)-norcamphor: influence of steric modifications of  
 the bicyclic framework on asymmetric sulfoxidation  
 AUTHOR(S): Lattanzi, Alessandra; Iannece, Patrizia; Scettri,  
 Arrigo  
 CORPORATE SOURCE: Dipartimento di Chimica, Universita degli Studi di  
 Salerno, Baronissi (SA), 84081, Italy  
 SOURCE: Tetrahedron: Asymmetry (2004), 15(11), 1779-1785  
 CODEN: TASYE3; ISSN: 0957-4166  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB A renewable tertiary hydroperoxide I has been efficiently synthesized in 83% overall yield starting from com. available (+)-endo-2-norborneol. This oxygen donor, derived from (+)-norcamphor, when employed in Ti(OCHMe<sub>2</sub>)<sub>4</sub>-catalyzed oxidns. of sulfides to sulfoxides, proved to be considerably more reactive when compared to a previously reported camphor-derived hydroperoxide. Reduced steric hindrance of the new oxidant lowered the level of asym. induction achieved in the oxidation, but stereoconvergent kinetic resolution has been exploited to improve

enantioselectivity. Excellent recovery (95%) of the tertiary alc., (+)-exo-2-furyl-2-norborneol, at the end of the oxidation provides a highly advantageous chiral resource saving protocol.

## RX(18) OF 20 - 3 STEPS



NOTE: 1) mol. sieves used, 3) stereoselective

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 139:164895 CASREACT

TITLE: Tremorgenic Indole Alkaloids. The Total Synthesis of (-)-Penitrem D

AUTHOR(S): Smith, Amos B.; Kanoh, Naoki; Ishiyama, Haruaki; Minakawa, Noriaki; Rainier, Jon D.; Hartz, Richard A.; Cho, Young Shin; Cui, Haifeng; Moser, William H.

CORPORATE SOURCE: Department of Chemistry, Monell Chemical Senses Center, and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, PA, 19104, USA

SOURCE: Journal of the American Chemical Society (2003), 125(27), 8228-8237

CODEN: JACSAT; ISSN: 0002-7863

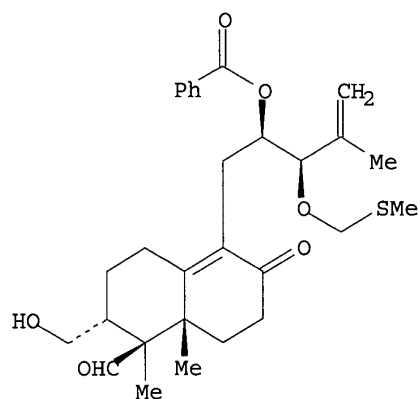
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

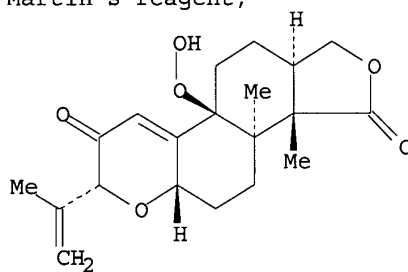
LANGUAGE: English

AB A convergent, stereocontrolled total synthesis of the architecturally complex tremorgenic indole alkaloid (-)-penitrem D was achieved. Highlights of the synthesis include an efficient, asym. synthesis of the western hemisphere; the stereocontrolled assembly of the I-ring; discovery of a novel autoxidn. to introduce the C(22) tertiary hydroxyl group, required for tremorgenic activity; union of fully elaborated eastern and western hemispheres, exploiting an indole synthetic protocol developed expressly for this purpose; and a late-stage, stereoselective construction of the A and F rings exploiting a Sc(OTf)<sub>3</sub>-promoted reaction cascade. The longest linear sequence leading to (-)-penitrem D was 43 steps.

## RX(450) OF 754 - 5 STEPS



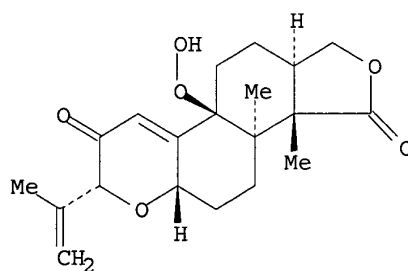
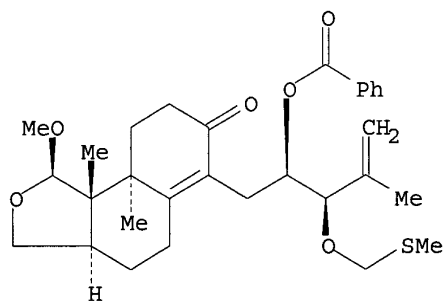
1. PDC, CH<sub>2</sub>Cl<sub>2</sub>
- 2.1. Et<sub>3</sub>SiH, F<sub>3</sub>CSO<sub>2</sub>H, PhMe
- 2.2. Et<sub>3</sub>N
- 3.1. K<sub>2</sub>CO<sub>3</sub>, MeOH, Water
- 3.2. HCl, Water
- 3.3. EDAP, 4-DMAP, CH<sub>2</sub>Cl<sub>2</sub>
4. Martin's reagent,



72%

NOTE: 2) stereoselective

## RX(452) OF 754 - 6 STEPS

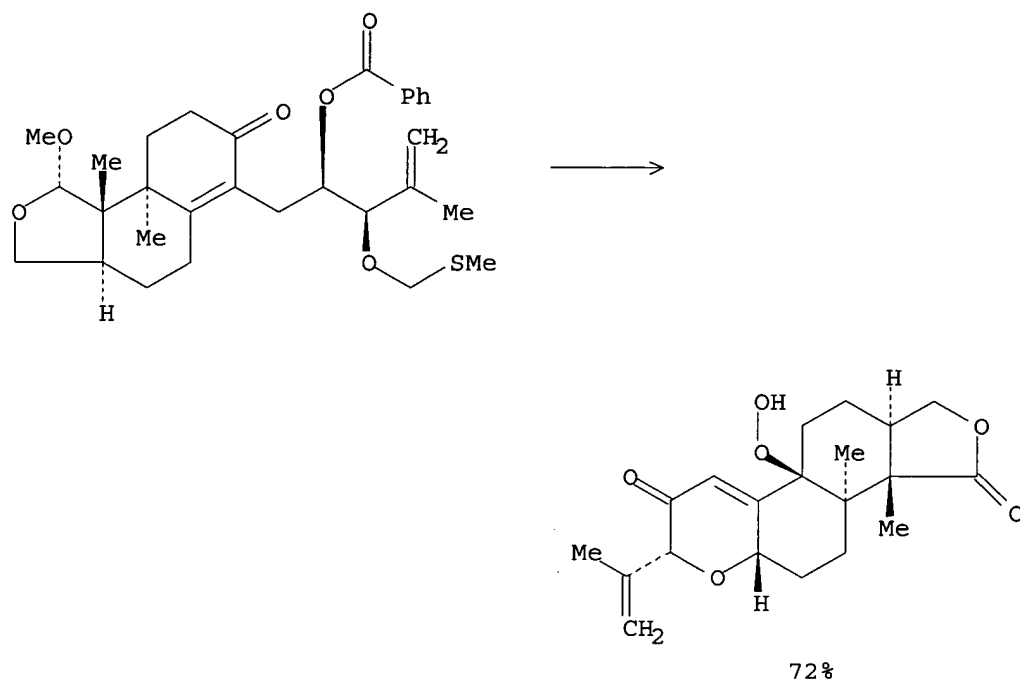


72%

NOTE: 3) stereoselective

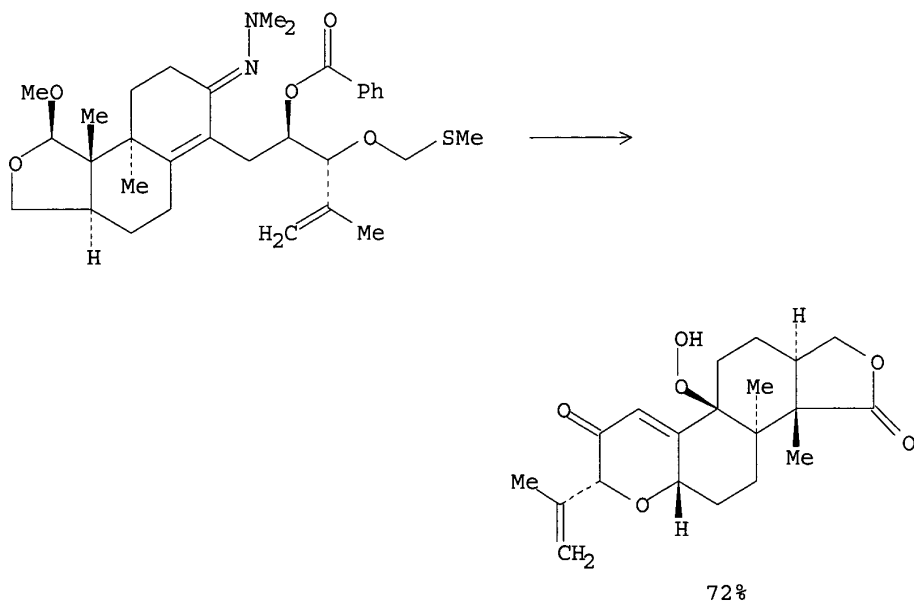


RX(454) OF 754 - 6 STEPS



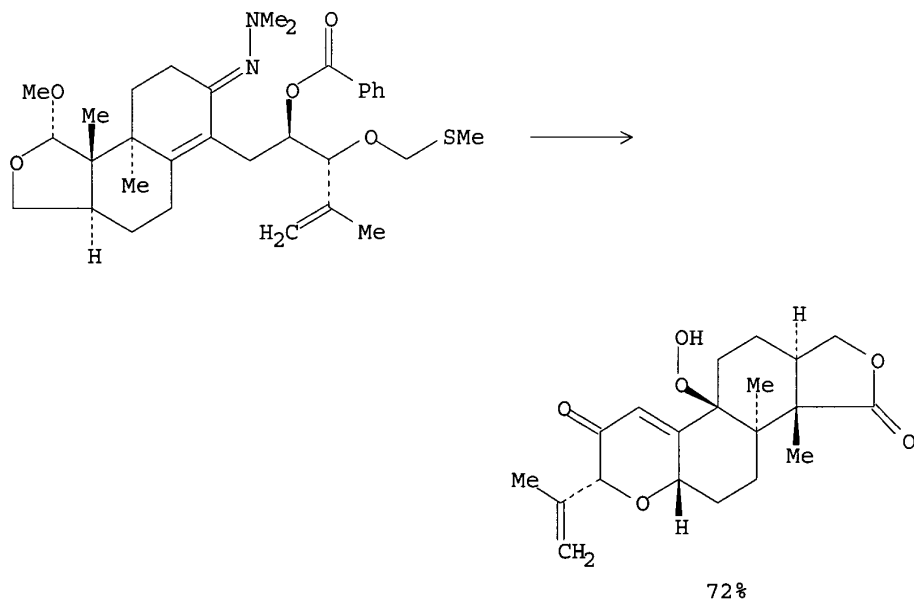
NOTE: 3) stereoselective

RX(456) OF 754 - 7 STEPS



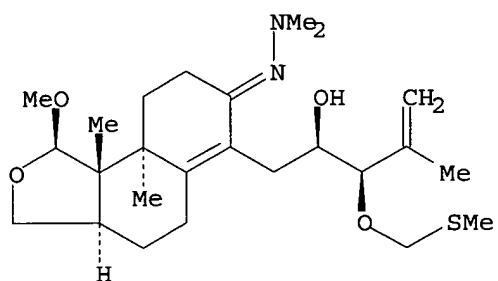
NOTE: 1) buffered soln. used first stage, 4) stereoselective

RX(458) OF 754 - 7 STEPS

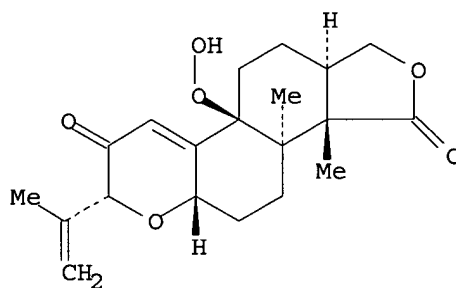


NOTE: 1) buffered soln. used first stage, 4) stereoselective

RX(580) OF 754 - 8 STEPS



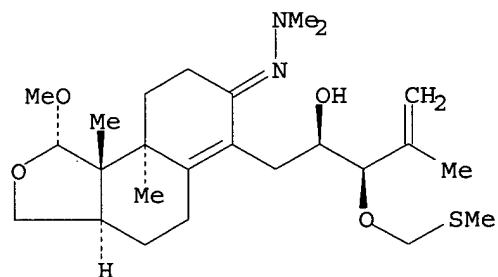
1. PhCOCl



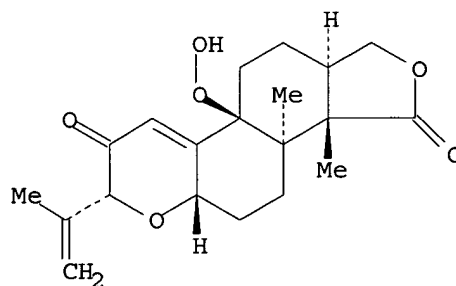
72%

NOTE: 2) buffered soln. used first stage, 5) stereoselective

RX(581) OF 754 - 8 STEPS



1.1. PhCOCl



72%

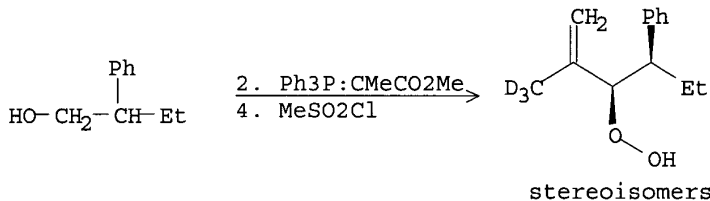
NOTE: 2) buffered soln. used first stage, 5) stereoselective

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 4 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 139:323158 CASREACT  
 TITLE: Remarkable Change of the Diastereoselection in the Dye-Sensitized Ene Hydroperoxidation of Chiral Alkenes by Zeolite Confinement  
 AUTHOR(S): Stratakis, Manolis; Kalaitzakis, Dimitris; Stavroulakis, Dimitris; Kosmas, Giannis; Tsangarakis, Constantinos  
 CORPORATE SOURCE: Department of Chemistry, University of Crete, Iraklion, 71409, Greece  
 SOURCE: Organic Letters (2003), 5(19), 3471-3474  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

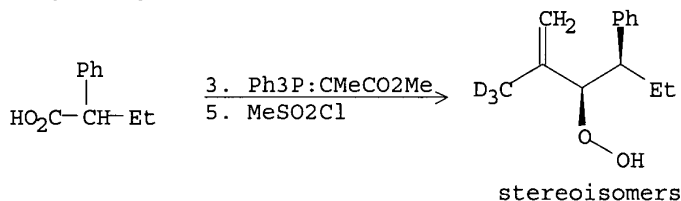
AB The ene reaction of singlet oxygen with chiral trisubstituted alkenes bearing an alkyl and a Ph group at the stereogenic center is erythro diastereoselective in solution and threo diastereoselective if carried out within zeolite Na-Y. The change of the diastereoselectivity trend by zeolite confinement is attributed to a synergism of steric effects and cation- $\pi$  interactions.

RX(72) OF 76 - 6 STEPS



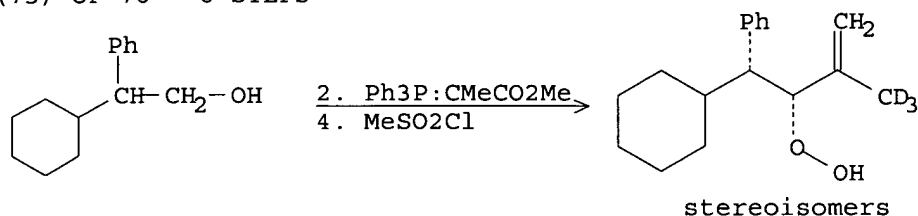
NOTE: 2) stereoselective, 6) regioselective, stereoselective, photochem., Na-Y zeolite used

RX(73) OF 76 - 7 STEPS



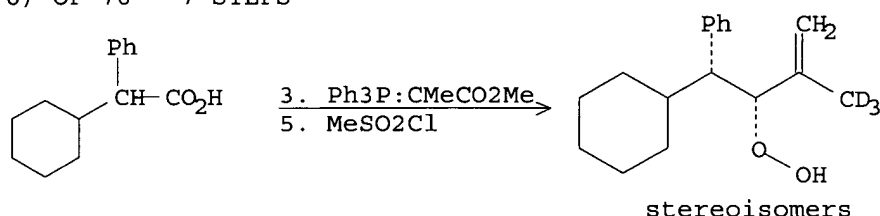
NOTE: 3) stereoselective, 7) regioselective, stereoselective, photochem., Na-Y zeolite used

## RX(75) OF 76 - 6 STEPS



NOTE: 2) stereoselective, 6) regioselective, stereoselective, photochem., Na-Y zeolite used

## RX(76) OF 76 - 7 STEPS



NOTE: 3) stereoselective, 7) regioselective, stereoselective, photochem., Na-Y zeolite used

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 5 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 139:133800 CASREACT

TITLE: Asymmetric synthesis with 6-tert-butyl-5-methoxy-6-methyl-3,6-dihydro-2H-1,4-oxazin-2-one as a new chiral glycine equivalent: preparation of enantiomerically pure  $\alpha$ -tertiary and  $\alpha$ -quaternary  $\alpha$ -amino acids

AUTHOR(S): Koch, Claus-Jurgen; Simonyiova, Sona; Pabel, Jorg; Kartner, Annerose; Polborn, Kurt; Wanner, Klaus Theodor

CORPORATE SOURCE: Department Pharmazie - Zentrum fur Pharmaforschung, LMU Munchen, Munchen, 81377, Germany

SOURCE: European Journal of Organic Chemistry (2003), (7), 1244-1263

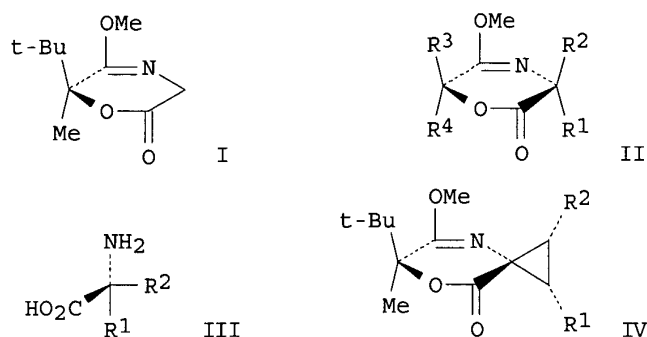
CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



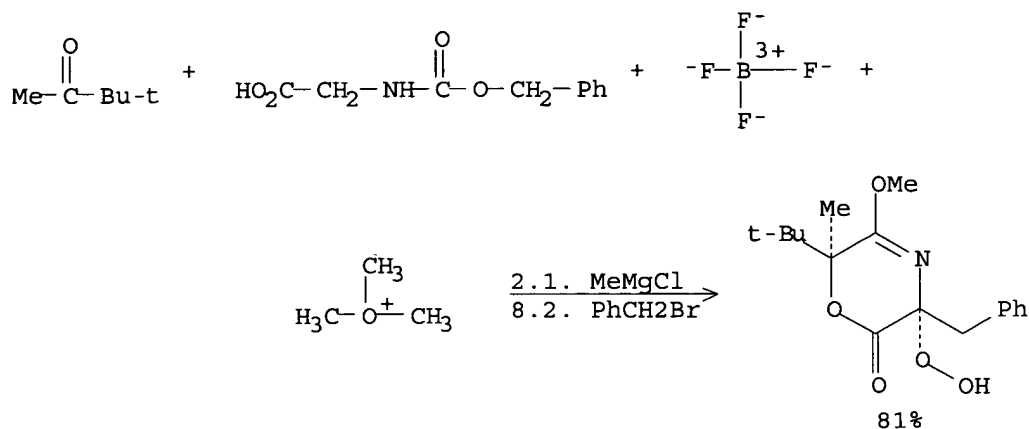
AB The chiral oxazinone I has been developed as a new chiral glycine equivalent for the asym. synthesis of mono- and disubstituted  $\alpha$ -amino acids.

It is derived from the  $\alpha$ -hydroxy-carboxylic acid, which serves as a chiral auxiliary, and is easily accessible in enantiomerically pure form by optical resolution of the racemic compound (RS)-2-hydroxy-2,3,3-trimethylbutanoic acid. For alkylation reactions, I was deprotonated with sBuLi or phosphazenic base. Subsequent treatment with alkyl halides yielded the monosubstituted compds. II (R1 = CH<sub>2</sub>Ph, CH<sub>2</sub>CH:CH<sub>2</sub>, Me, n-Bu, iso-Pr, R2 = H, R3 = tert-Bu, R4 = Me; R1 = H, R2 = CH<sub>2</sub>Ph, CH<sub>2</sub>CH:CH<sub>2</sub>, Me, n-Bu, i-Pr; R3 = tert-Bu, R4 = Me) and (ent)-II (R1 = H, R2 = 13CH<sub>3</sub>, R3 = Me, R4 = t-Bu; R1 = 13CH<sub>3</sub>, R2 = H, R3 = Me, R4 = t-Bu), while a second alkylation step, via the corresponding enolates, provided the disubstituted compds. II (R1 = CH<sub>2</sub>CH:CH<sub>2</sub>, Me, n-Bu, iso-Pr, R2 = CH<sub>2</sub>Ph, R3 = tert-Bu, R4 = Me; R1 = CH<sub>2</sub>Ph, R2 = CH<sub>2</sub>CH:CH<sub>2</sub>, Me, n-Bu, iso-Pr, R3 = tert-Bu, R4 = Me). Both alkylation steps proceeded with good yields and excellent diastereoselectivities (up to 99% de) and even less reactive electrophiles such as iso-Pr iodide could be used. The results obtained in this reaction supported the assumption that the enolate of I, as well as those of the monosubstituted derivs. of I, have less tendency to form the aggregates that hamper alkylation reactions with other systems with higher oxygen content. From the major diastereomers of both the mono- and the disubstituted derivs. of I the corresponding  $\alpha$ -amino acids III (R1 = CH<sub>2</sub>Ph, CH<sub>2</sub>CH:CH<sub>2</sub>, Me, R2 = H; R1 = CH<sub>2</sub>CH:CH<sub>2</sub>, Me, n-Bu, iso-Pr, R2 = CH<sub>2</sub>Ph) were obtained in high enantiomeric purity by hydrolytic cleavage of the oxazinone ring, accomplished either in two steps with aqueous TFA and

aqueous

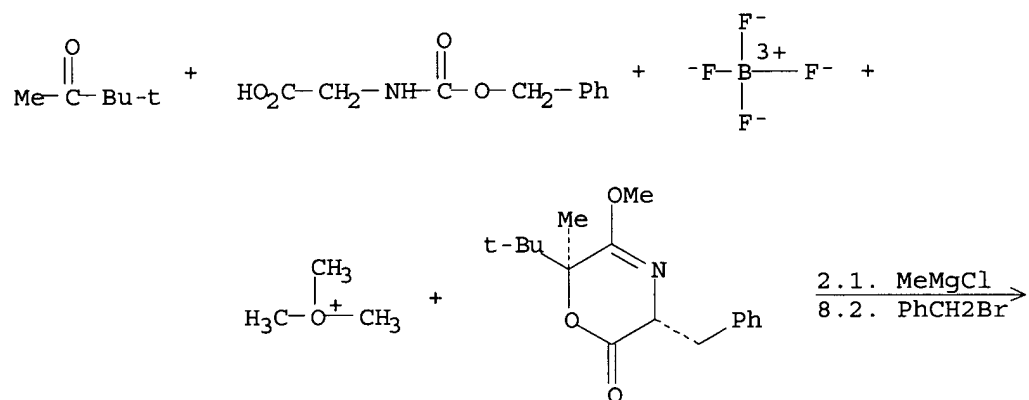
NaOH or in one with either aqueous NaOH or 3 N HBr. Alkylation of the enolate ions of (S)-I or (R)-I with epichlorohydrins as bifunctional electrophiles provided the hydroxymethylenecyclopropyl derivs. IV (R1 = CH<sub>2</sub>OH, R2 = H; R1 = H, R2 = CH<sub>2</sub>OH). Hydrolysis of IV (R1 = CH<sub>2</sub>OH, R2 = H; R1 = H, R2 = CH<sub>2</sub>OH) afforded the free (1R,2S)- and (1R,2R)-1-amino-2-(hydroxymethyl)cyclopropanecarboxylic acids. Reductive amination with aniline after oxidation of IV (R1 = CH<sub>2</sub>OH, R2 = H; R1 = H, R2 = CH<sub>2</sub>OH) to the corresponding aldehydes provided the compds. IV (R1 = CH<sub>2</sub>NHPh, R2 = H; R1 = H, R2 = CH<sub>2</sub>NHPh), whereas Mitsunobu treatment of IV (R1 = CH<sub>2</sub>OH, R2 = H; R1 = H, R2 = CH<sub>2</sub>OH) with 1-phenyl-3-(trifluoroacetyl)urea afforded the urea derivs. Hydrolysis of these compds. yielded the (1R,2R)- and (1S,2S)-1-amino-2-(phenylaminomethyl)cyclopropanecarboxylic acids, and (1R,2R)-1-amino-2-(aminomethyl)cyclopropanecarboxylic acid.

RX(665) OF 750 - 9 STEPS

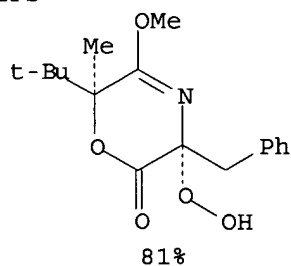


NOTE: 3) stereoselective, 7) buffered soln. used stage 2, 8) stereoselective, yields depend on reaction conditions, 9) buffered soln. used stage 3

RX(693) OF 750 - 10 STEPS



RX(693) OF 750 - 10 STEPS



NOTE: 3) stereoselective, 7) buffered soln. used stage 2, 8) stereoselective, yields depend on reaction conditions, 10) buffered soln. used stage 3

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 6 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 138:55585 CASREACT

TITLE: Thionin-Sensitized Intrazeolite Photooxygenation of Trisubstituted Alkenes: Substituent Effects on the Regioselectivity As Probed through Isotopic Labeling

AUTHOR(S): Stratakis, Manolis; Nencka, Radim; Rabalakos, Constantinos; Adam, Waldemar; Krebs, Oliver

CORPORATE SOURCE: Department of Chemistry, University of Crete, Iraklion, 71409, Greece

SOURCE: Journal of Organic Chemistry (2002), 67(25), 8758-8763  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

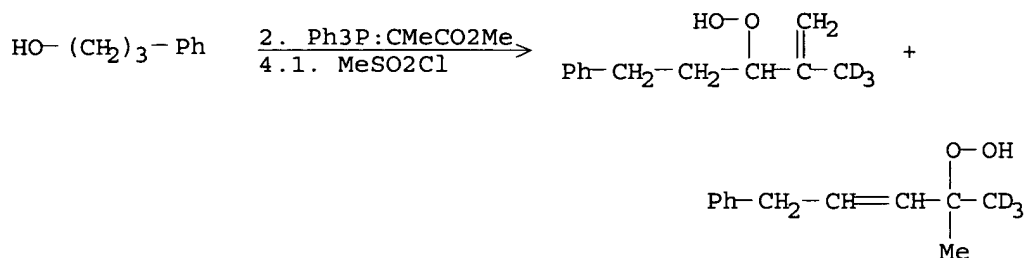
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The regioselectivity for the intrazeolite photooxygenation of several trisubstituted alkenes with geminal di-Me groups was examined. The length of the alkyl chain at the lone position was varied, and as end groups, the Ph or the cyclohexyl functionalities were chosen. The general trend for all alkenes is a significant increase of the reactivity at the twin position compared to the photooxygenation in solution. For the cyclohexyl-substituted alkenes, it was found that the regioselectivity is nearly independent of the alkyl chain length. However, for the phenyl-substituted alkenes, the ene reactivity of the allylic methylene hydrogen atoms at the lone position and the twix/twin regioselectivity depend significantly on the distance of the Ph group from the double bond. These trends are discussed in terms of cation- $\pi$  interactions and conformational effects. Intramol. and intermol. isotope effects in the intrazeolite photooxygenation of deuterium-labeled alkenes suggest that a perepoxide-type intermediate is formed in the rate-determining step. Type I photooxygenation that involves reaction of the radical cations of the alkenes with superoxide ion are unlikely.

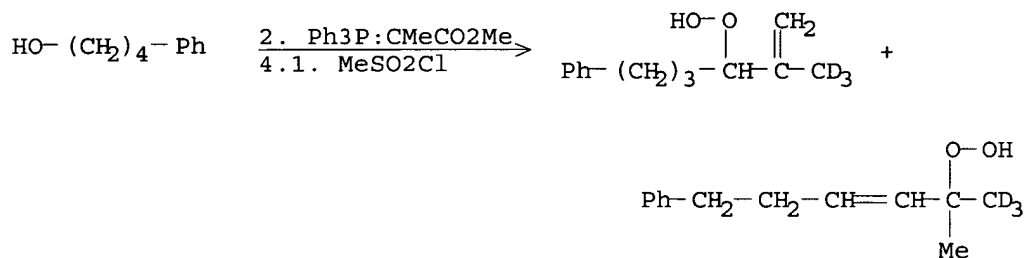


RX(126) OF 141 - 6 STEPS



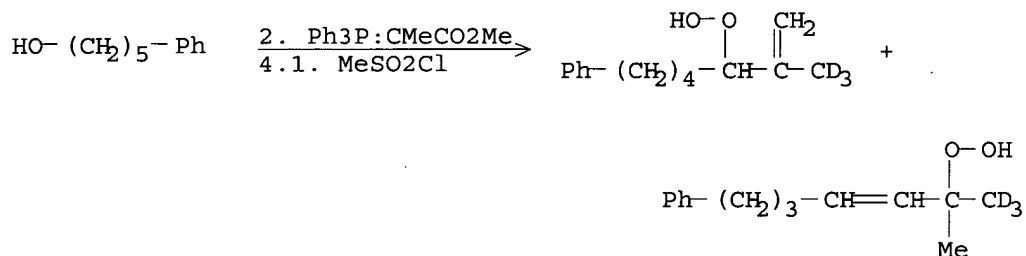
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

RX(129) OF 141 - 6 STEPS



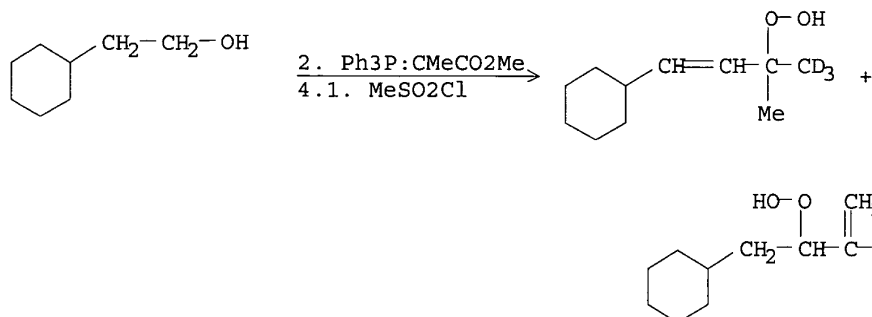
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

RX(132) OF 141 - 6 STEPS



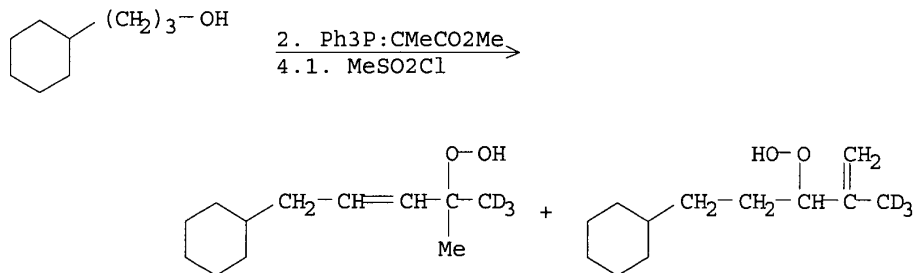
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

## RX(135) OF 141 - 6 STEPS



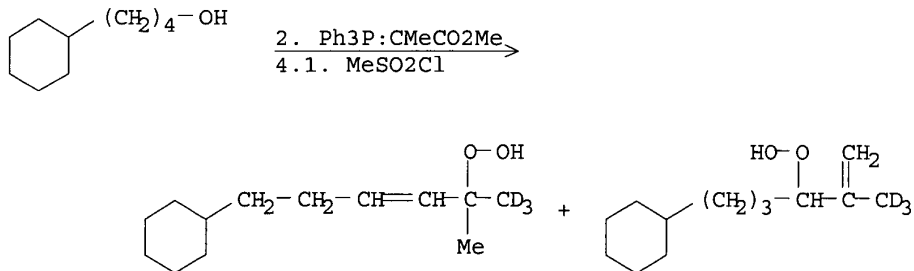
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

## RX(138) OF 141 - 6 STEPS



NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

## RX(141) OF 141 - 6 STEPS



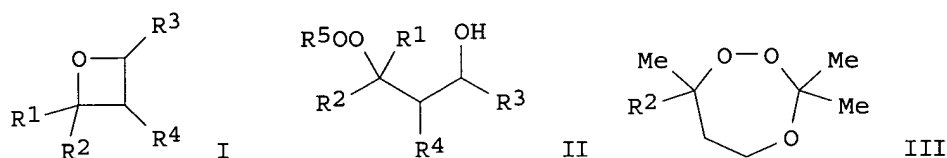
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

REFERENCE COUNT:

23

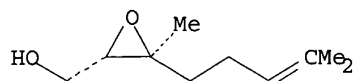
THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 7 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 138:137276 CASREACT  
 TITLE: Opening of Substituted Oxetanes with H<sub>2</sub>O<sub>2</sub> and Alkyl Hydroperoxides: Stereoselective Approach to 3-Peroxyalcohols and 1,2,4-Trioxepanes  
 AUTHOR(S): Dussault, Patrick H.; Trullinger, Tony K.; Noor-e-Ain, Farhana  
 CORPORATE SOURCE: Department of Chemistry, University of Nebraska Lincoln, Lincoln, NE, 68588-0304, USA  
 SOURCE: Organic Letters (2002), 4(26), 4591-4593  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

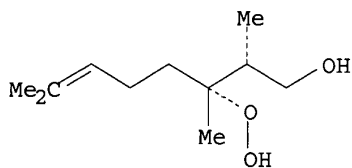


AB Lewis acid-catalyzed ring opening of optically active oxetanes I [R1 = R3 = R4 = H, R2 = n-hexyl; R1 = Me, R2 = n-C<sub>16</sub>H<sub>33</sub>, Me<sub>2</sub>C:CHCH<sub>2</sub>CH<sub>2</sub>, Me<sub>2</sub>CH(CH<sub>2</sub>)<sub>3</sub>; R3, R4 = H, Me] by hydrogen peroxide proceeded regioselectively and with good to moderate stereoselectivity to furnish enantiomerically enriched 3-hydroperoxyalkanols II (R5 = H). The analogous opening using alkyl hydroperoxides R5O<sub>2</sub>H (R5 = Me<sub>3</sub>C, cumyl, tetrahydropyranyl) furnished the corresponding 3-peroxyalkanols II. II (R1 = Me; R2 = n-C<sub>16</sub>H<sub>33</sub>, Me<sub>2</sub>C:CHCH<sub>2</sub>CH<sub>2</sub>; R3 = R4 = R5 = H) were easily converted into enantiomerically enriched 1,2,4-trioxepanes III, the building blocks for antimalarials.

## RX(65) OF 76 - 3 STEPS



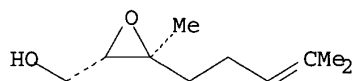
- 1.1. MeLi, CuI, Et<sub>2</sub>O
- 1.2. NH<sub>4</sub>Cl, Water
- 2.1. t-BuOK, TsCl, THF
- 2.2. t-BuOK
- 3.1. C:54761-04-5, H<sub>2</sub>O<sub>2</sub>
- 3.2. 2,6-Di-t-butylcresol, Water, AcOEt



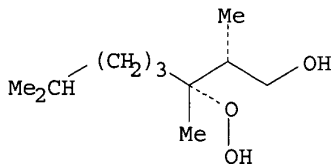
81%

NOTE: 1) stereoselective, 3) regioselective, stereoselective, yield depends on reaction conditions

## RX(69) OF 76 - 4 STEPS



- 1.1. MeLi, CuI, Et<sub>2</sub>O
- 1.2. NH<sub>4</sub>Cl, Water
2. Pd, H<sub>2</sub>, EtOH
- 3.1. t-BuOK, TsCl, THF
- 3.2. t-BuOK
- 4.1. C:54761-04-5, H<sub>2</sub>O<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>
- 4.2. 2,6-Di-t-butylcresol, Water, AcOEt



46%

NOTE: 1) stereoselective, 4) regioselective, stereoselective, product depends on reaction conditions

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

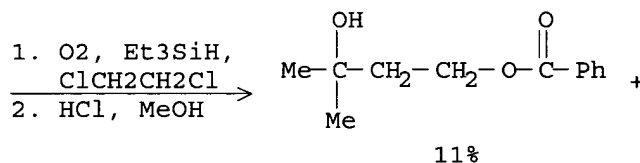
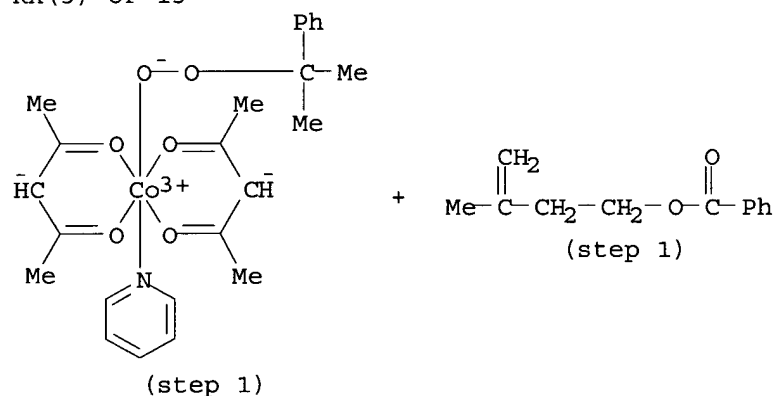
L34 ANSWER 8 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 138:4635 CASREACT  
 TITLE: Co(III)-Alkyl Complex- and Co(III)-Alkylperoxo  
 Complex-Catalyzed Triethylsilylperoxidation of Alkenes  
 with Molecular Oxygen and Triethylsilane

AUTHOR(S): Tokuyasu, Takahiro; Kunikawa, Shigeki; Masuyama, Araki; Nojima, Masatomo  
 CORPORATE SOURCE: Department of Materials Chemistry Frontier Research Center Graduate School of Engineering, Osaka University, Osaka, 565-0871, Japan  
 SOURCE: Organic Letters (2002), 4(21), 3595-3598  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

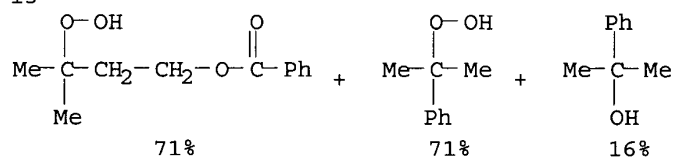
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Both a Co(III)-alkyl complex and a Co(III)-alkylperoxo complex catalyze triethylsilylperoxidn. of alkenes with O<sub>2</sub> and Et<sub>3</sub>SiH. E.g., Co(modp)<sub>2</sub> (bis(1-(morpholinocarbamoyl)-4,4-dimethyl-1,3-pentanedionato)cobalt(II)) (shown as I) or Co(acac)<sub>2</sub> (II)-catalyzed peroxidn. of H<sub>2</sub>C:C(CH<sub>3</sub>)(CH<sub>2</sub>)<sub>2</sub>OCOPh proceeded regioselectively affording the triethylsilyl peroxide Et<sub>3</sub>SiOOC(CH<sub>3</sub>)<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>OCOPh in high yield. Although less efficient, cobalt(II) Schiff base complex [Co(SB)] (shown as III) also catalyzed the same reaction. On this basis, together with the non-stereoselectivity in the Co(II)-catalyzed peroxidn. of 3-phenylindene and the formation of the corresponding 1,2-dioxolane from 2-phenyl-1-vinylcyclopropane (a radical clock), the authors propose a reasonable mechanism for the Co(II)-catalyzed novel autoxidn. of alkenes with Et<sub>3</sub>SiH discovered by Isayama and Mukaiyama.

RX(3) OF 13

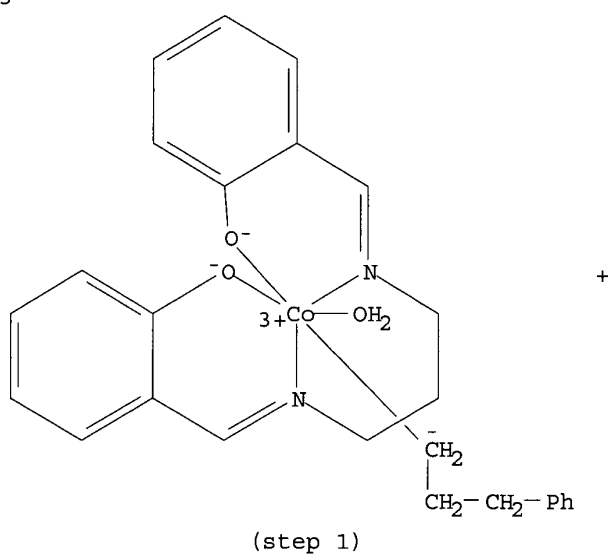


RX(3) OF 13

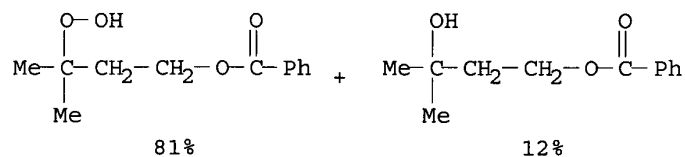
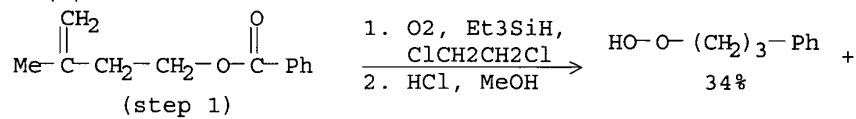


NOTE: room temp., 3 h

RX(6) OF 13

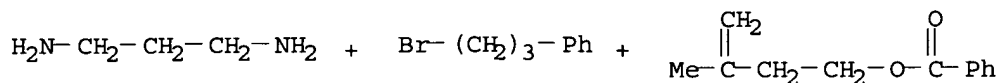


RX(6) OF 13



NOTE: regioselective, room temp., 3.5 h

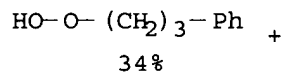
RX(13) OF 13 - 2 STEPS

1.1. 2-HOC<sub>6</sub>H<sub>4</sub>CHO,

MeOH

1.2. R:7791-13-1

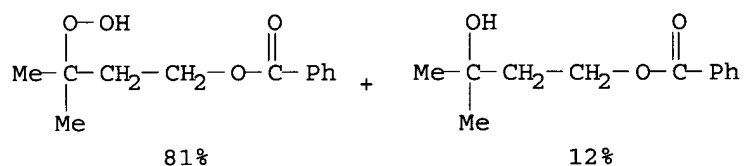
1.3. NaOH, Water

1.4. PdCl<sub>2</sub>, KCl,NaBH<sub>4</sub>, Water

34%

2.1. O<sub>2</sub>, Et<sub>3</sub>SiH,ClCH<sub>2</sub>CH<sub>2</sub>Cl

2.2. HCl, MeOH



NOTE: 2) regioselective, room temp., 3.5 h

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 9 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 136:386270 CASREACT

TITLE: A concise synthesis of an advanced clerodin intermediate through a Vaultier tandem reaction

AUTHOR(S): Lallemand, Jean-Yves; Six, Yvan; Ricard, Louis

CORPORATE SOURCE: Laboratoire DCSO. URA 1308 du CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.

SOURCE: European Journal of Organic Chemistry (2002), (3), 503-513

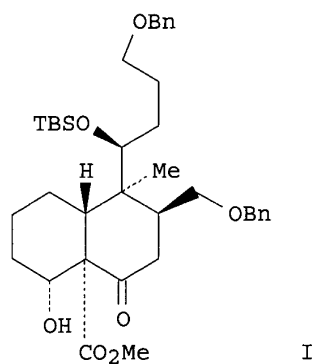
CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

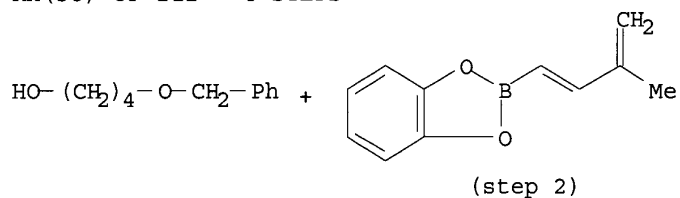
LANGUAGE: English

GI

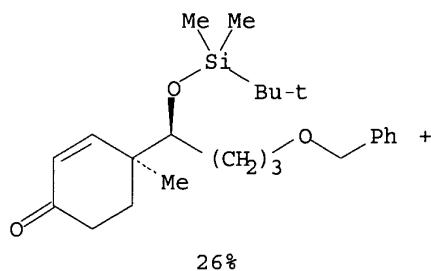


AB A highly functionalized precursor (I) of the antifeedant natural product clerodin has been synthesized with good diastereo-control. Key steps include a three-component version of the Vaultier tandem sequence, and an oxidative decarboxylation with a simple exptl. procedure.

RX(58) OF 212 - 4 STEPS

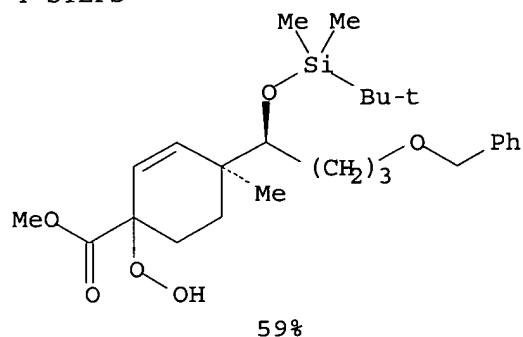


1. PDC, CH<sub>2</sub>Cl<sub>2</sub>
2. Me acrylate
3. F<sub>3</sub>CSO<sub>3</sub>SiMe<sub>2</sub>Bu-t,  
2,6-Lutidine,  
CH<sub>2</sub>Cl<sub>2</sub>
- 4.1. O<sub>2</sub>, THF
- 4.2. t-BuOK, THF



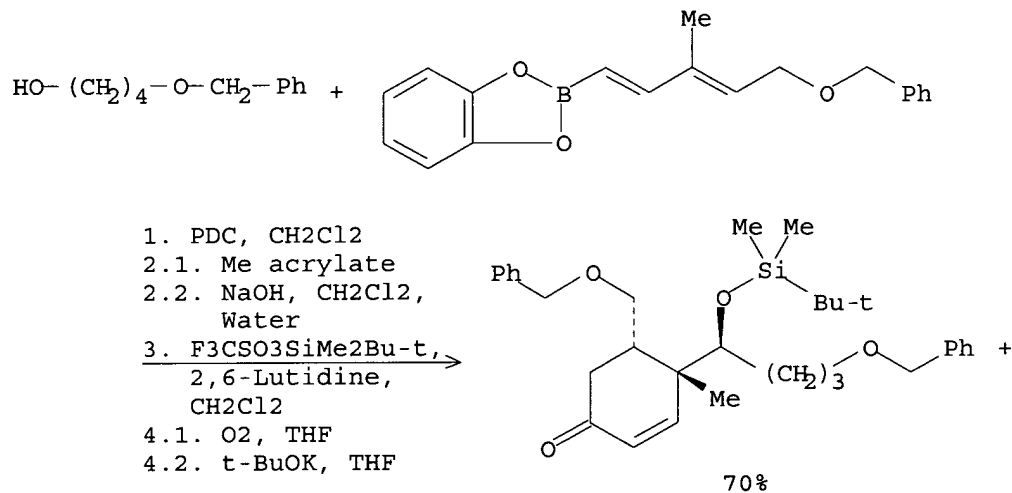


RX(58) OF 212 - 4 STEPS

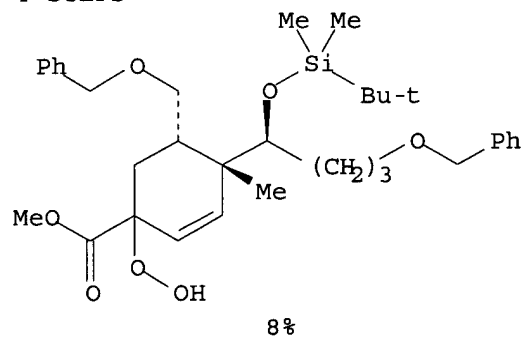


NOTE: 1) Celite used, 2) alternative reaction conditions gave lower yield

RX(66) OF 212 - 4 STEPS

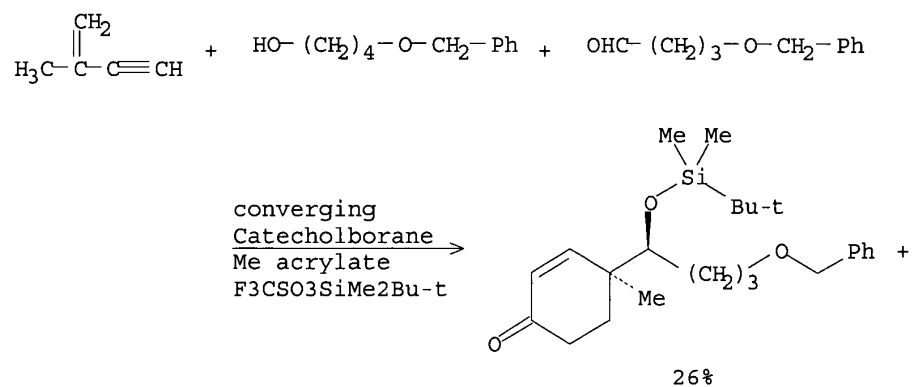


RX(66) OF 212 - 4 STEPS

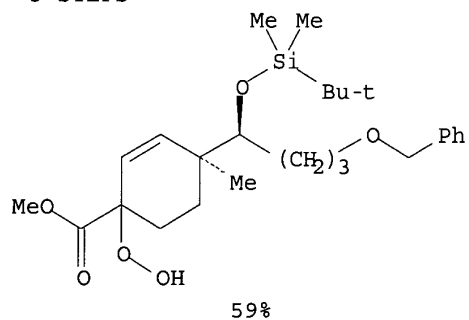


NOTE: 1) Celite used, 2) petroleum ether solvent used

RX(103) OF 212 - 5 STEPS

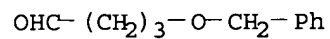
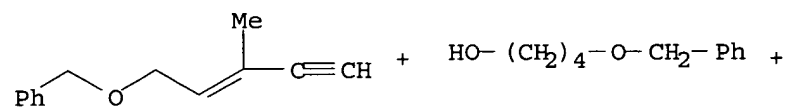


RX(103) OF 212 - 5 STEPS

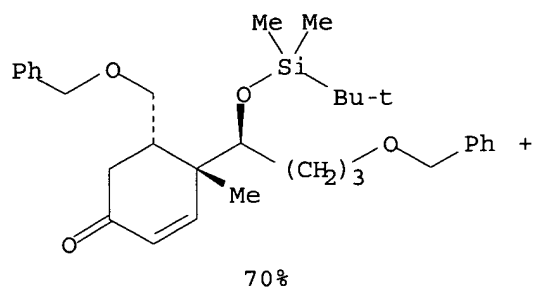


NOTE: alternative reaction conditions gave lower yield, Celite used

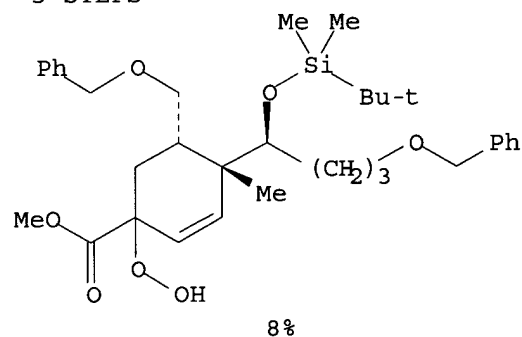
RX(139) OF 212 - 5 STEPS



converging  
Catecholborane  
Me acrylate  
Me acrylate  
F3CSO3SiMe2Bu-t

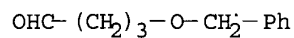
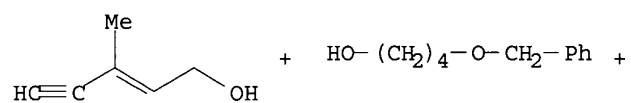


RX(139) OF 212 - 5 STEPS

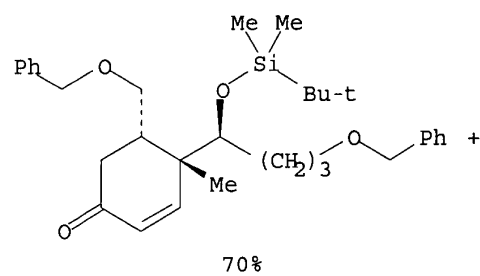


NOTE: petroleum ether solvent used, Celite used

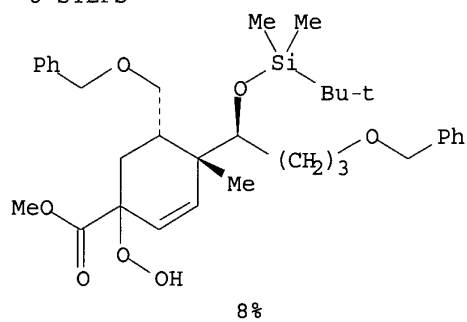
RX(145) OF 212 - 6 STEPS



converging  
 PhCH<sub>2</sub>Br  
 Catecholborane  
 Me acrylate  
 Me acrylate  
 F<sub>3</sub>CSO<sub>3</sub>SiMe<sub>2</sub>Bu-t

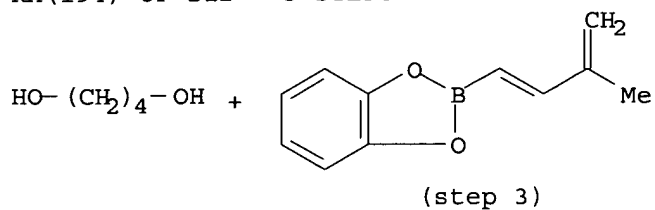


RX(145) OF 212 - 6 STEPS

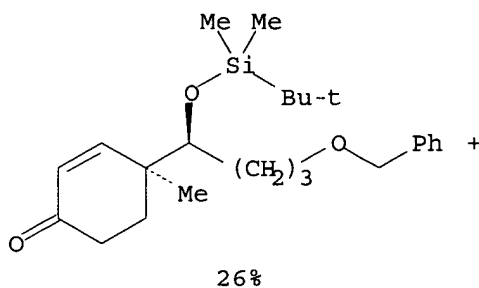


NOTE: petroleum ether solvent used, Celite used

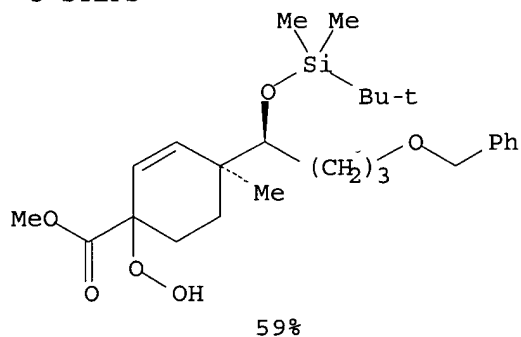
RX(194) OF 212 - 5 STEPS



- 1.1. NaH, THF
- 1.2. PhCH<sub>2</sub>Br, Bu<sub>4</sub>N.I., THF
2. PDC, CH<sub>2</sub>Cl<sub>2</sub>
3. Me acrylate
4. F<sub>3</sub>CSO<sub>3</sub>SiMe<sub>2</sub>Bu-t, 2,6-Lutidine, CH<sub>2</sub>Cl<sub>2</sub>
- 5.1. O<sub>2</sub>, THF
- 5.2. t-BuOK, THF

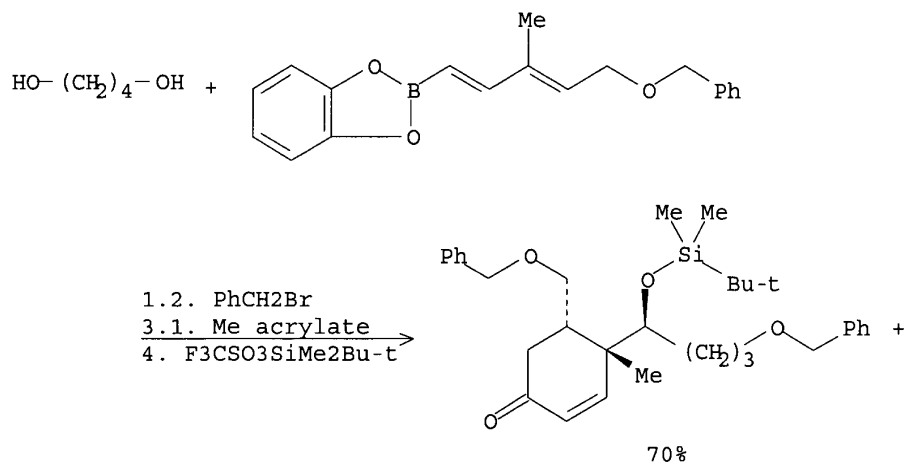


RX(194) OF 212 - 5 STEPS

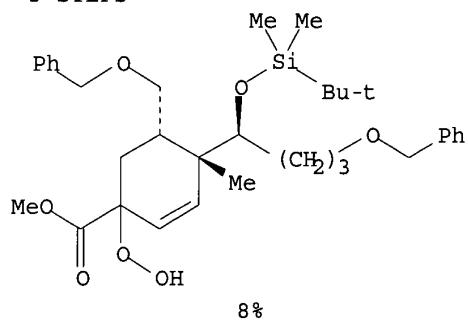


NOTE: 2) Celite used, 3) alternative reaction conditions gave lower yield

RX(195) OF 212 - 5 STEPS

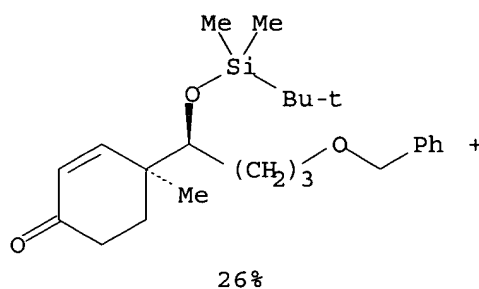
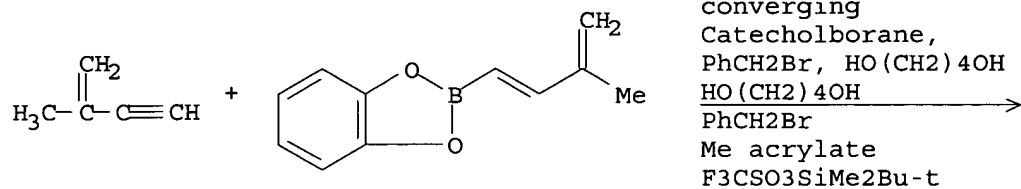


RX(195) OF 212 - 5 STEPS

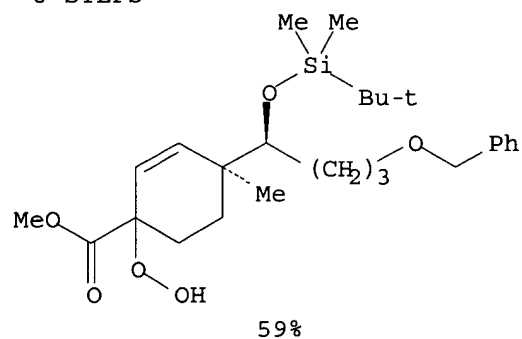


NOTE: 2) Celite used, 3) petroleum ether solvent used

RX(197) OF 212 - 6 STEPS

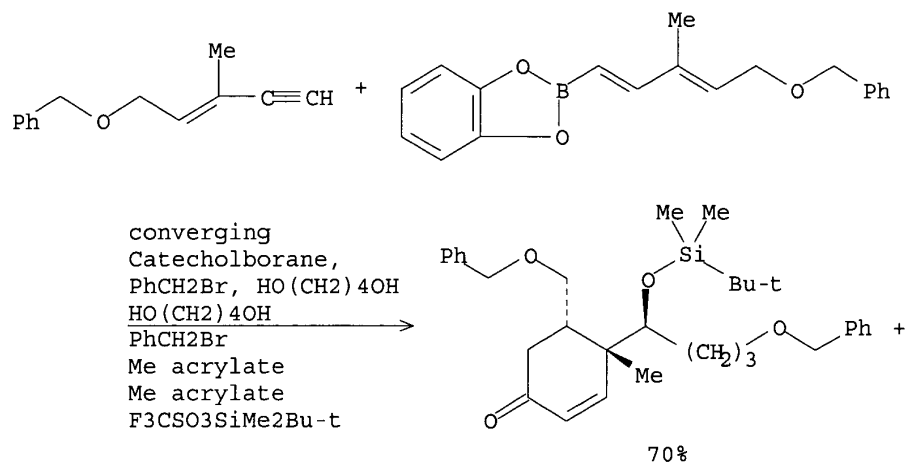


RX(197) OF 212 - 6 STEPS

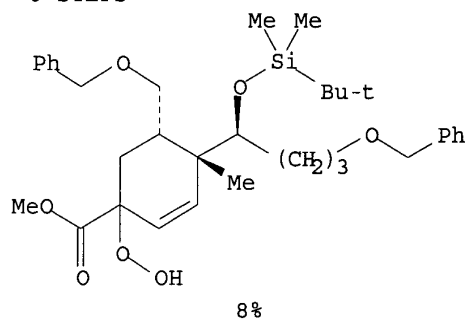


NOTE: Celite used, alternative reaction conditions gave lower yield

RX(198) OF 212 - 6 STEPS

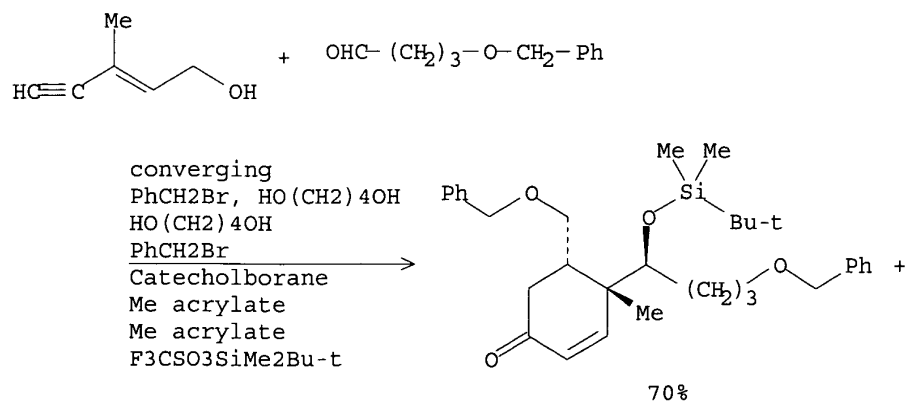


RX(198) OF 212 - 6 STEPS



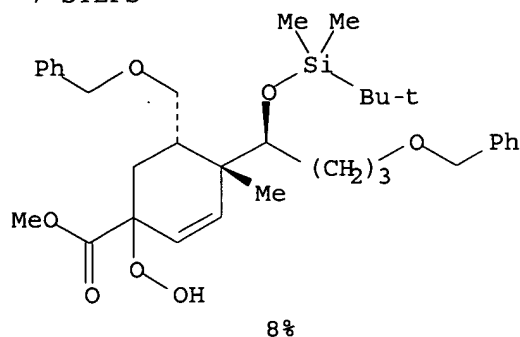
NOTE: Celite used, petroleum ether solvent used

RX(212) OF 212 - 7 STEPS





RX(212) OF 212 - 7 STEPS



NOTE: petroleum ether solvent used, Celite used

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 10 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 127:161309 CASREACT

TITLE: Chemoselective oxidation of organozinc reagents with oxygen

AUTHOR(S): Klement, Ingo; Lutjens, Henning; Knochel, Paul

CORPORATE SOURCE: Fachbereich Chemie Philipps-Univ., Marburg, D-35032, Germany

SOURCE: Tetrahedron (1997), 53(27), 9135-9144

CODEN: TETRAB; ISSN: 0040-4020

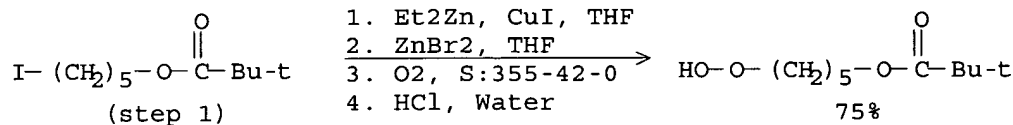
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

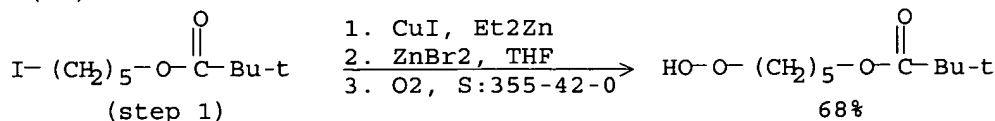
LANGUAGE: English

AB Functionalized organozinc compds., prepared by hydrozincation, carbozincation or by boron-zinc exchange, can be directly oxidized in a selective manner to the corresponding functionalized alcs. or hydroperoxides depending on the reaction conditions.

RX(34) OF 42



RX(42) OF 42



NOTE: safety, pyrophoric reagent, intermediate products could be isolated, chemoselective

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 11 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 126:144478 CASREACT

TITLE: New optically pure sugar hydroperoxides. Synthesis and use for enantioselective oxygen transfer

AUTHOR(S): Hamann, Hans-Juergen; Hoeft, Eugen; Mostowicz, Danuta; Mishnev, Anatoly; Urbanczyk-Lipkowska, Zofia; Chmielewski, Marek

CORPORATE SOURCE: Inst. Chemistry, Humboldt Univ., Berlin, Germany

SOURCE: Tetrahedron (1997), 53(1), 185-192

CODEN: TETRAB; ISSN: 0040-4020

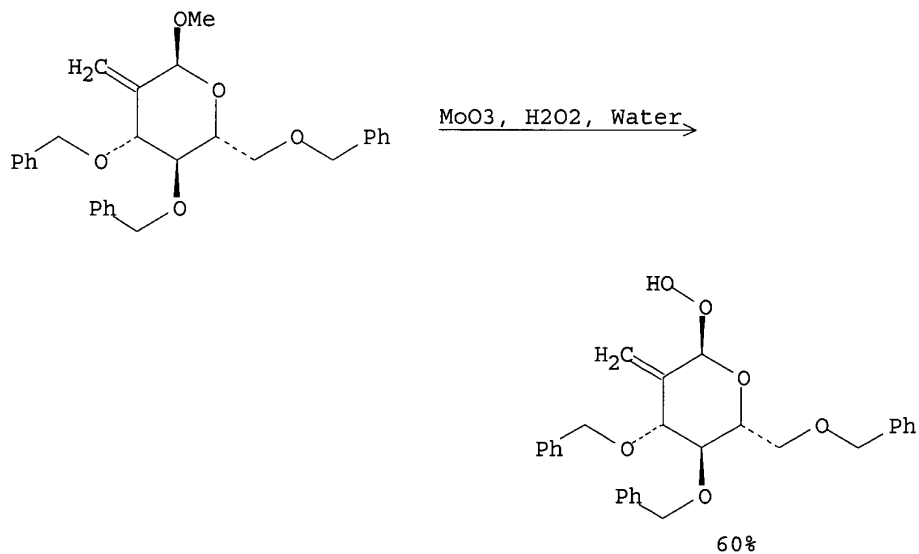
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 2-Deoxy-2-C-methylene Me glycosides undergo oxidation with hydrogen peroxide in the presence of molybdenum trioxide as catalyst to afford the corresponding anomeric hydroperoxides. These hydroperoxides were used as chiral oxidants of allylic alcs. and prochiral sulfides to offer moderate enantioselectivities which were, however, higher than those reported before for oxidation with optically active peroxyacids.

RX(1) OF 3



NOTE: enantioselective, key step

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

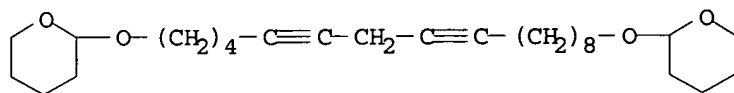
L34 ANSWER 12 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 122:239362 CASREACT

TITLE: A Chemoenzymic Approach to Hydroperoxyeicosatetraenoic Acids. Total Synthesis of 5(S)-HPETE  
 AUTHOR(S): Dussault, Patrick; Lee, In Quen  
 CORPORATE SOURCE: Department of Chemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA  
 SOURCE: Journal of Organic Chemistry (1995), 60(1), 218-26  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A new synthetic approach to enantiomerically pure hydroperoxyeicosatetraenoic acids (HPETEs) is described in which the tetraene skeleton is assembled through chemoselective olefination of a protected hydroperoxy aldehyde. Soybean lipooxygenase-mediated dioxygenation of both natural and unnatural fats produces hydroperoxy dienes in high enantiomeric excess; the observed regioselectivity supports a revised hypothesis for substrate specificity. Protection of the diene hydroperoxides as peroxy ketals is followed by regioselective ozonolysis to afford enantiomerically pure 4-peroxy 2,3-enals which undergo olefination to produce peroxytetraenoates. Removal of the monoperoxy ketal and the Me ester affords enantiomerically pure HPETEs. The generality of the strategy is illustrated with the first chemical synthesis of 5(S)-HPETE, 5(S)-hydroperoxy-(6E,8Z,11Z,14Z)-eicosatetraenoic acid.

RX(146) OF 337 - 3 STEPS



1.1. Ni(OAc)<sub>2</sub>, H<sub>2</sub>,  
NaBH<sub>4</sub>, EtOH,  
Water

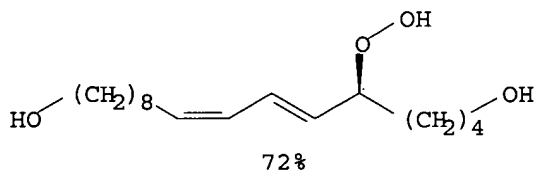
1.2. H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>,  
EtOH

2.1. p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H.H<sub>2</sub>O,  
MeOH

2.2. Na<sub>2</sub>CO<sub>3</sub>, Water

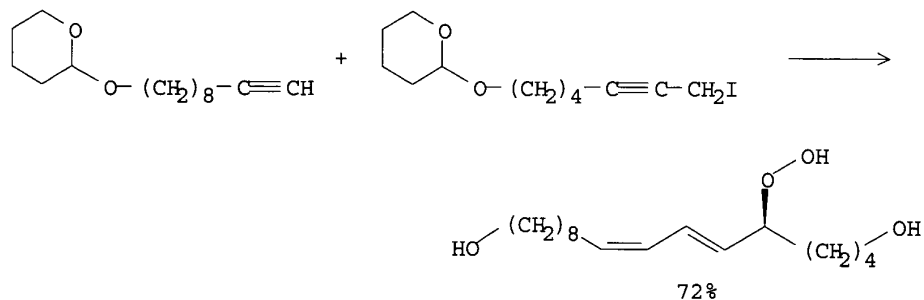
3.1. O<sub>2</sub>, Water, EtOH

3.2. 2,6-Di-t-butylcresol,



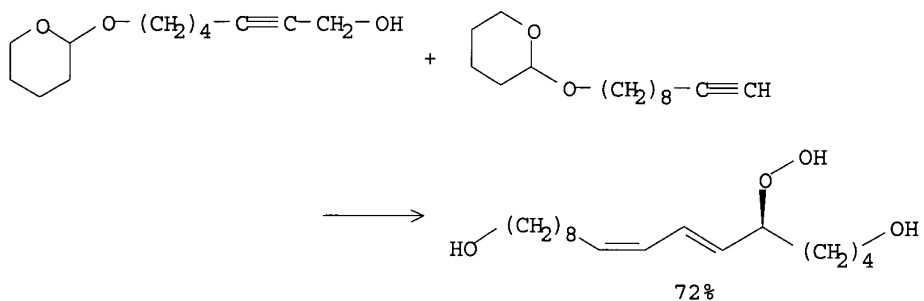
NOTE: 1) stereoselective, 3) stereoselective, biotransformation, enzymic, soybean type I lipooxygenase used, buffered soln.

## RX(149) OF 337 - 4 STEPS



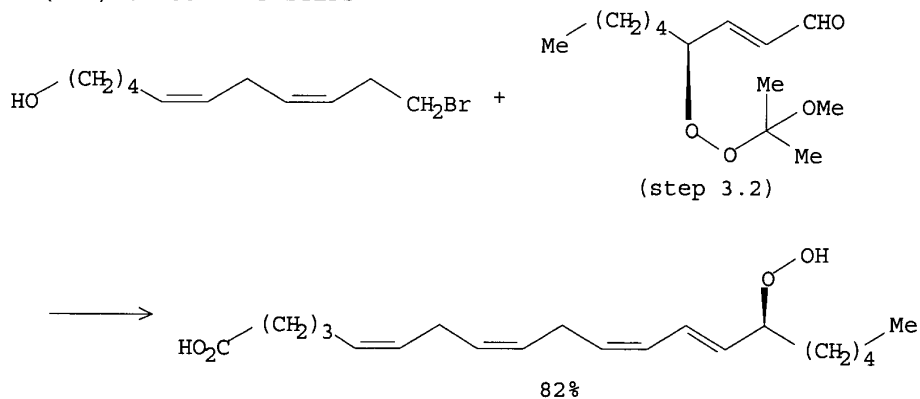
NOTE: 2) stereoselective, 4) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

## RX(172) OF 337 - 5 STEPS



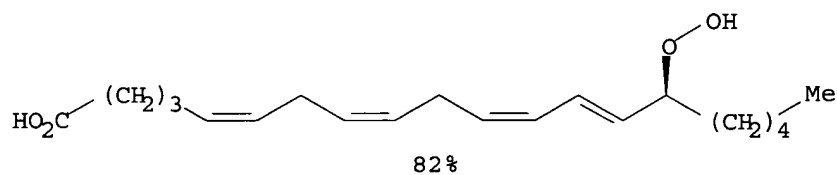
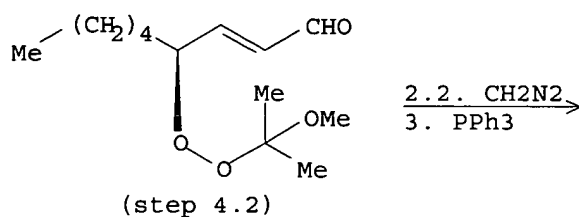
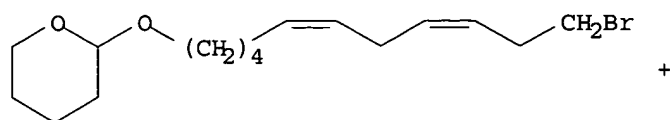
NOTE: 3) stereoselective, 5) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

## RX(188) OF 337 - 5 STEPS



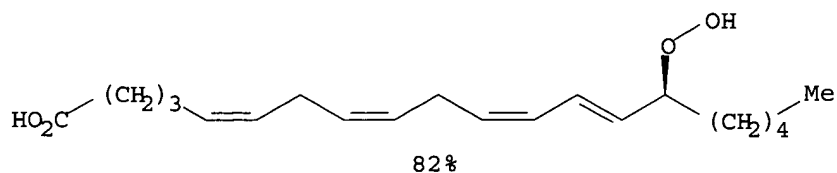
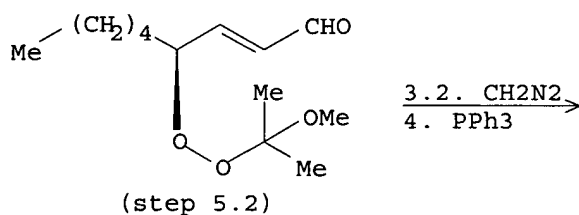
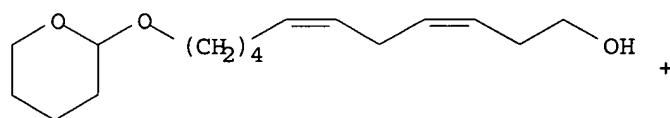
NOTE: 2) no exptl. detail, 3) stereoselective, Wittig olefination, key step, 4) safety-peroxides (BHT used), 5) safety-peroxides (BHT used)

RX(190) OF 337 - 6 STEPS



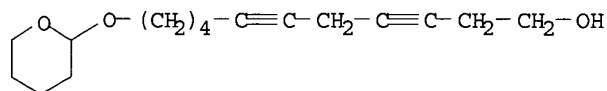
NOTE: 3) no exptl. detail, 4) stereoselective, Wittig olefination, key step, 5) safety-peroxides (BHT used), 6) safety-peroxides (BHT used)

RX(192) OF 337 - 7 STEPS

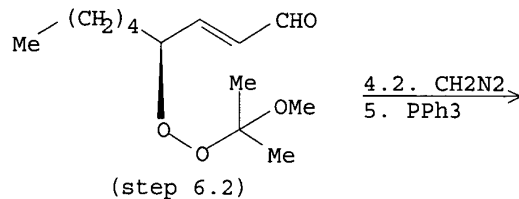


NOTE: 4) no exptl. detail, 5) stereoselective, Wittig olefination, key step, 6) safety-peroxides (BHT used), 7) safety-peroxides (BHT used)

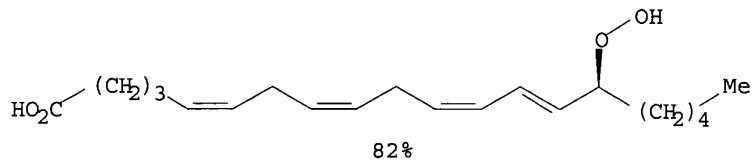
RX(194) OF 337 - 8 STEPS



+

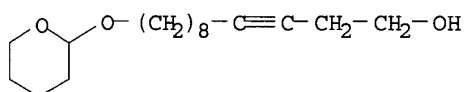


4.2.  $\text{CH}_2\text{N}_2$   
5.  $\text{PPh}_3$

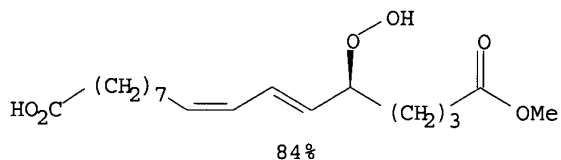


NOTE: 1) stereoselective, 5) no exptl. detail, 6) stereoselective, Wittig olefination, key step, 7) safety-peroxides (BHT used), 8) safety-peroxides (BHT used)

RX(218) OF 337 - 7 STEPS

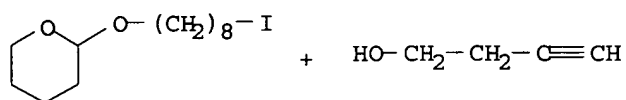


3.  $\text{PPh}_3$   
4.2.  $\text{HC}(\text{O})(\text{CH}_2)_3\text{CO}_2\text{Me}$

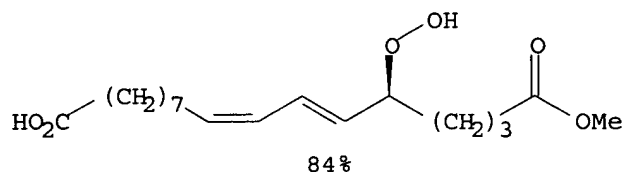


NOTE: 1) stereoselective, 4) stereoselective, Wittig olefination, key step, 6) Jones reagent used, 7) biotransformation, enzymic, soybean type I lipxygenase used, buffered soln.

RX(219) OF 337 - 8 STEPS

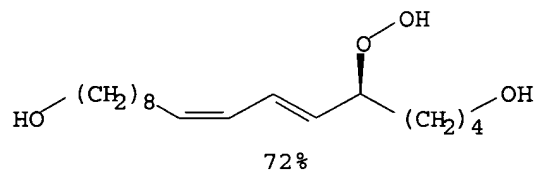
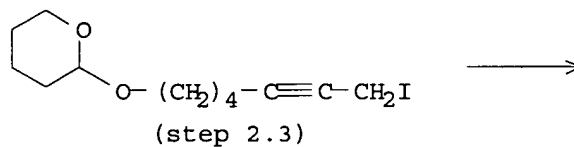
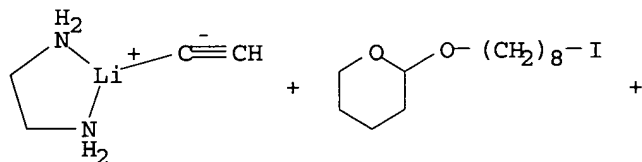


4. PPh<sub>3</sub>  
 5.2. HC(O)(CH<sub>2</sub>)<sub>3</sub>CO<sub>2</sub>Me



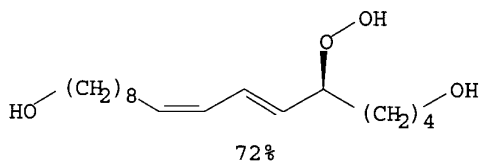
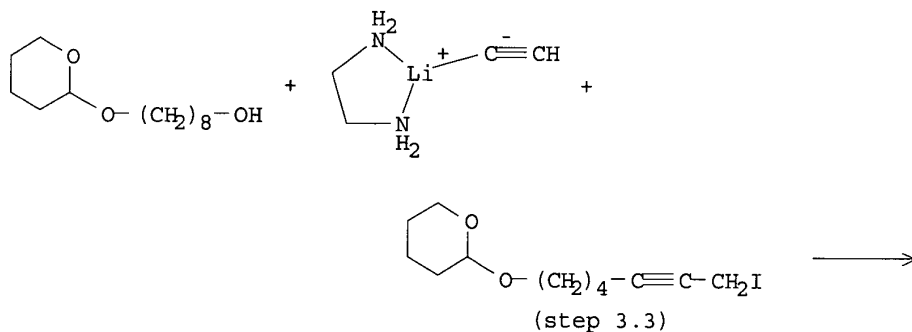
NOTE: 1) regioselective, 2) stereoselective, 5) stereoselective, Wittig olefination, key step, 7) Jones reagent used, 8) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(249) OF 337 - 5 STEPS



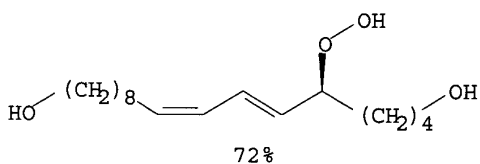
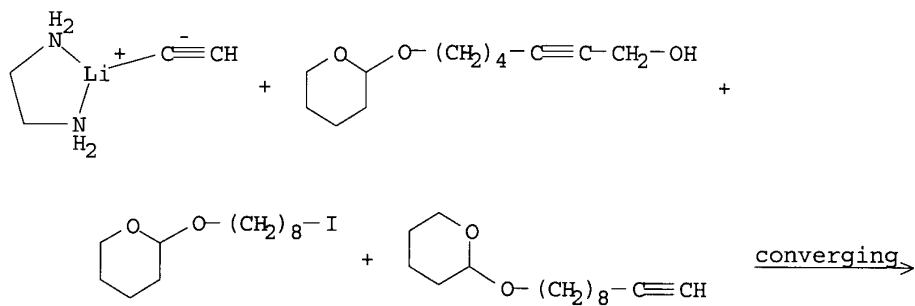
NOTE: 3) stereoselective, 5) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

## RX(253) OF 337 - 6 STEPS



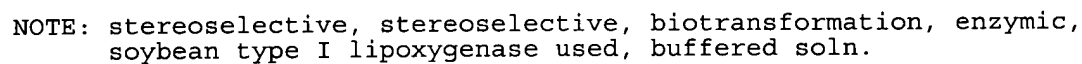
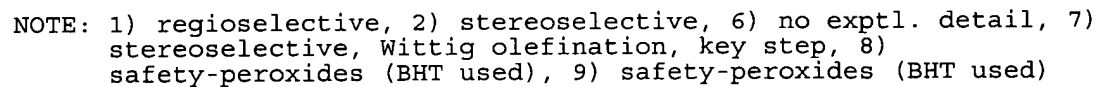
NOTE: 4) stereoselective, 6) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

## RX(256) OF 337 - 6 STEPS

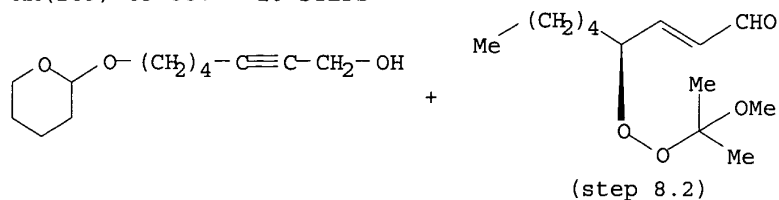


NOTE: stereoselective, stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

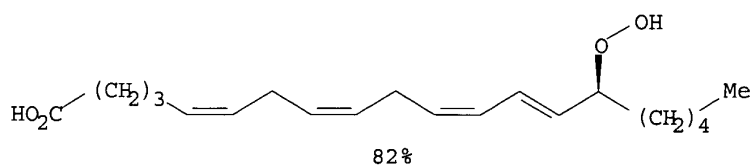


$$\text{C}_6\text{H}_{10}\text{O}(\text{CH}_2)_8\text{OH} + \text{C}_6\text{H}_{10}\text{O}(\text{CH}_2)_4\text{C}\equiv\text{CCH}_2\text{OH} +$$

$$\text{Cyclohexyl-O-(CH}_2\text{)}_4\text{-C}\equiv\text{C-CH}_2\text{I} + \text{HO-CH}_2\text{-CH}_2\text{-C}\equiv\text{CH} +$$


RX(289) OF 337 - 10 STEPS

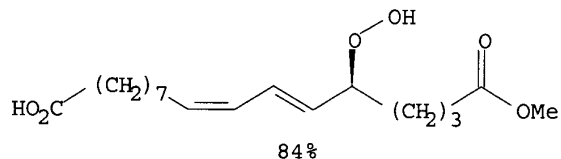
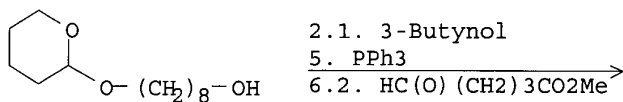


2.1. 3-Butynol  
 6.2. CH<sub>2</sub>N<sub>2</sub>  
 7. PPh<sub>3</sub>



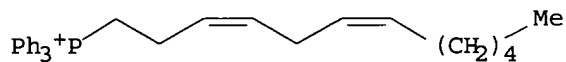
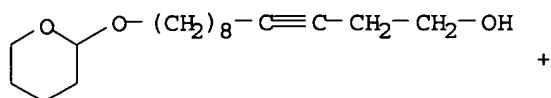
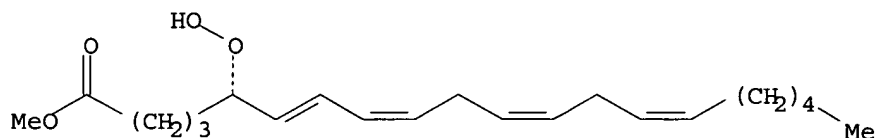
NOTE: 2) regioselective, 3) stereoselective, 7) no exptl. detail, 8) stereoselective, Wittig olefination, key step, 9) safety-peroxides (BHT used), 10) safety-peroxides (BHT used)

RX(290) OF 337 - 9 STEPS



NOTE: 2) regioselective, 3) stereoselective, 6) stereoselective, Wittig olefination, key step, 8) Jones reagent used, 9) biotransformation, enzymic, soybean type I lipxygenase used, buffered soln.

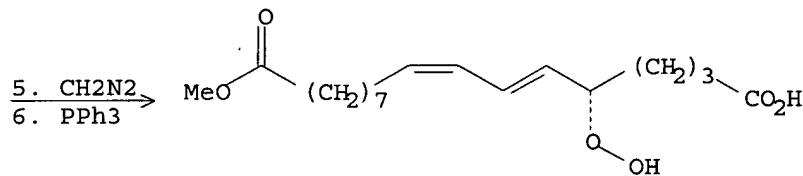
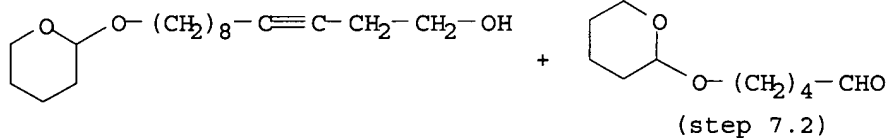
RX(306) OF 337 - 10 STEPS

3. PPh<sub>3</sub>4.2.  $\text{HC}(\text{O})(\text{CH}_2)_3\text{CO}_2\text{Me}$ 8.1.  $\text{H}_2\text{C}:\text{CMeOMe}$ Br<sup>-</sup>

93%

NOTE: 1) stereoselective, 4) stereoselective, Wittig olefination, key step, 6) Jones reagent used, 7) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln., 9) stereoselective, Wittig olefination, key step, 10) safety-peroxides (BHT used)

RX(307) OF 337 - 10 STEPS

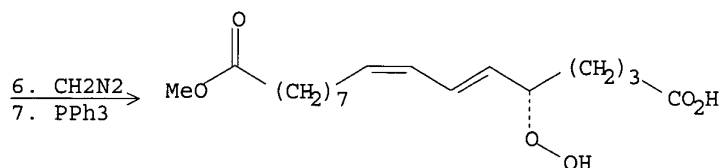
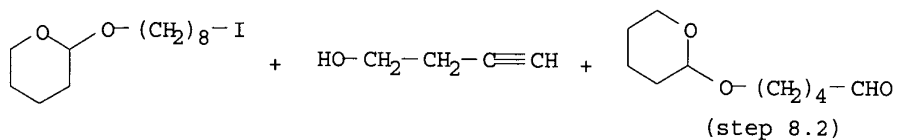


3%

NOTE: 1) stereoselective, 4) Jones reagent used, 7) stereoselective, Wittig olefination, key step, 9) Jones reagent used, 10) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

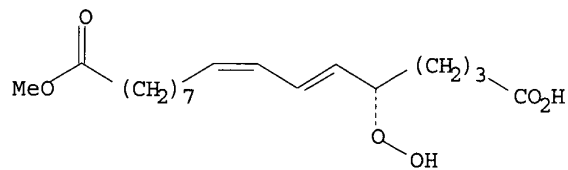
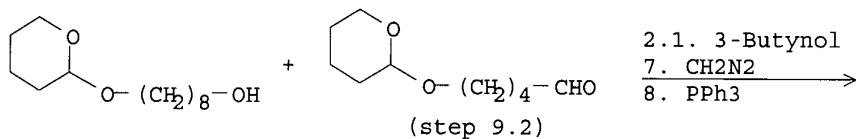
RX(309) OF 337 - 11 STEPS



NOTE: 1) regioselective, 2) stereoselective, 5) Jones reagent used, 8) stereoselective, Wittig olefination, key step, 10) Jones reagent used, 11) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

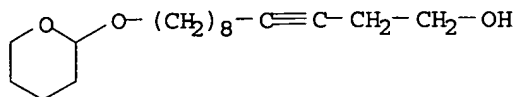
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(311) OF 337 - 12 STEPS

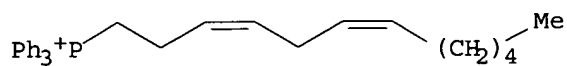


NOTE: 2) regioselective, 3) stereoselective, 6) Jones reagent used, 9) stereoselective, Wittig olefination, key step, 11) Jones reagent used, 12) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(319) OF 337 - 11 STEPS



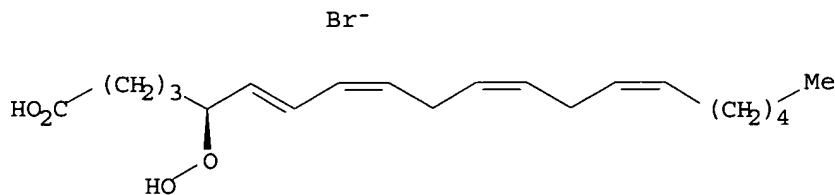
+



3. PPh3

4.2. HC(O)(CH2)3CO2Me

8.1. H2C:CMeOMe



83%

NOTE: 1) stereoselective, 4) stereoselective, Wittig olefination, key step, 6) Jones reagent used, 7) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln., 9) stereoselective, Wittig olefination, key step, 10) safety-peroxides (BHT used), 11) safety-peroxides (BHT used)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L34 ANSWER 13 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 116:106138 CASREACT

TITLE: Mercury(II)-mediated cyclization of hydroperoxyalkylcyclopropanes: a new route to cyclic peroxides

AUTHOR(S): Bloodworth, A. J.; Korkodilos, Despoina

CORPORATE SOURCE: Chem. Dep., Univ. Coll. London, London, WC1H 0AJ, UK

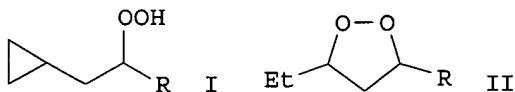
SOURCE: Tetrahedron Letters (1991), 32(47), 6953-6

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

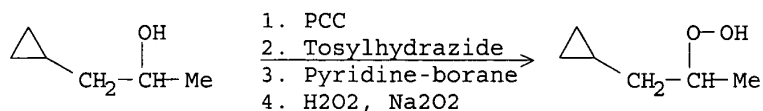
GI



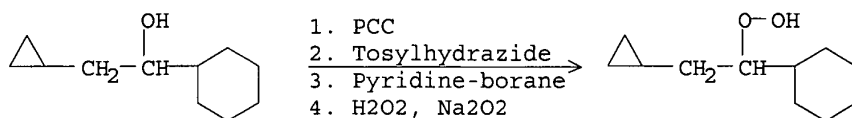
AB Aldehydes, RCHO (R = Me, Et, iso-Pr, cyclohexyl), have been converted via alkylation, cyclopropanation, oxidation, condensation with p-tosylhydrazine, reduction and perhydrolysis into 2-hydroperoxyalkylcyclopropanes I, and thence

by cycloperoxymercuration and reductive demercuration into the corresponding 3-alkyl-5-ethyl-1,2-dioxolanes II (R = Me, Et, iso-Pr, cyclohexyl).

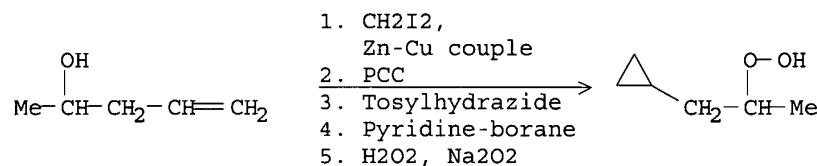
## RX(42) OF 72 - 4 STEPS



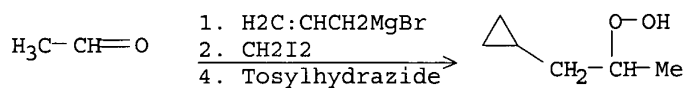
## RX(44) OF 72 - 4 STEPS



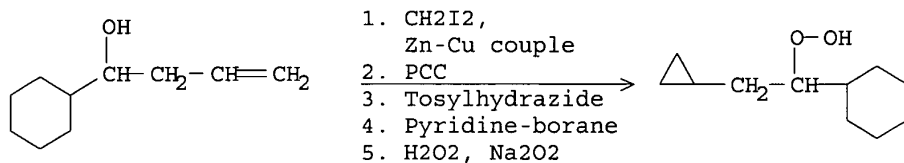
## RX(55) OF 72 - 5 STEPS



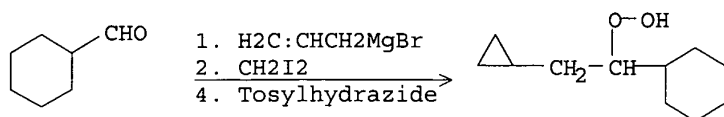
## RX(56) OF 72 - 6 STEPS



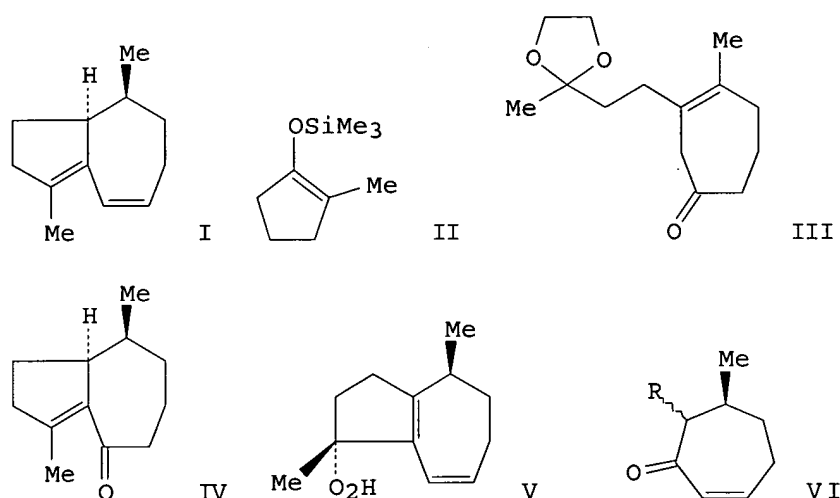
## RX(57) OF 72 - 5 STEPS



## RX(58) OF 72 - 6 STEPS

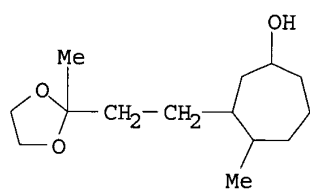


L34 ANSWER 14 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 115:256412 CASREACT  
 TITLE: Total synthesis of (±)-clavukerin A: a new  
 trinorguaiane sesquiterpene. Biomimetic synthesis of  
 (±)-clavularin A from (±)-clavukerin A  
 AUTHOR(S): Kim, Sung Kee; Pak, Chwang Siek  
 CORPORATE SOURCE: Korea Res. Inst. Chem. Technol., Daejeon, S. Korea  
 SOURCE: Journal of Organic Chemistry (1991), 56(24), 6829-32  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

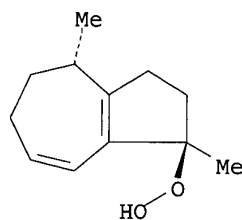


AB (±)-Clavukerin A (I) was synthesized in 8 steps starting from silyl enol ether II in 36% overall yield. The key elements of this synthesis are formation of substituted  $\beta,\gamma$ -unsatd. cycloheptenone III making using of the previously reported methodol. and highly stereoselective catalytic hydrogenation of III by Rh/alumina followed by acid-catalyzed cyclization to the hydroazulene skeleton IV. The Shapiro reaction was adopted for transformation of enone IV to I. Photooxidn. of I afforded an unstable hydroperoxide, (±)-clavukerin (V), which underwent rearrangement with acid to give (±)-clavularin A and B (VI; R =  $\alpha$ -CH<sub>2</sub>CH<sub>2</sub>COMe  $\beta$ -CH<sub>2</sub>CH<sub>2</sub>COMe; resp). Thus, this methodol. can be utilized as a general method for the preparation of the hydroazulene skeleton.

## RX(47) OF 60 - 5 STEPS



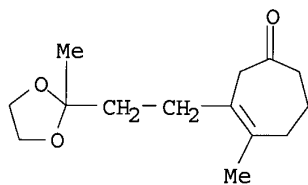
1. PDC, CH<sub>2</sub>Cl<sub>2</sub>
2. HCl, EtOH
3. Tosylhydrazide,  
HCl, MeOH
4. TMEDA, MeLi, THF,  
Hexane
5. Methylene blue, O<sub>2</sub>,  
MeOH, Pyridine



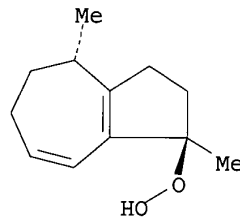
stereoisomers  
79%

NOTE: 5) Photochem.

## RX(49) OF 60 - 6 STEPS



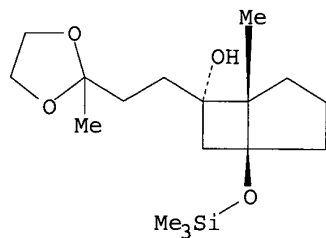
4. Tosylhydrazide



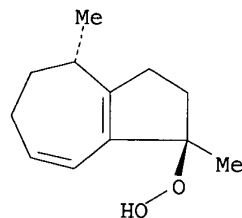
stereoisomers  
79%

NOTE: 1) Stereoselective, 6) Photochem.

## RX(51) OF 60 - 7 STEPS



5. Tosylhydrazide

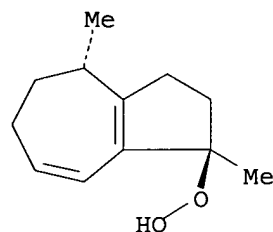
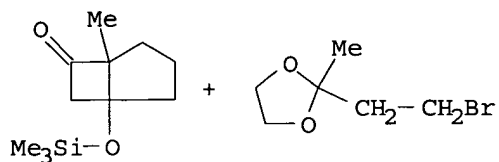


stereoisomers  
79%

NOTE: 1) Key step, 2) Stereoselective, 7) Photochem.



RX(52) OF 60 - 8 STEPS



stereoisomers

79%

NOTE: 1) stereoselective, 2) Key step, 3) Stereoselective, 8) Photochem.

L34 ANSWER 15 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 113:212359 CASREACT

TITLE: Stereocontrolled total synthesis of  
(±)-ptaquilosin, the aglycone of ptaquiloside, a  
bracken carcinogen

AUTHOR(S): Kigoshi, Hideo; Sawada, Akihiko; Nakayama, Yoshisuke;  
Niwa, Haruki; Yamada, Kiyoyuki

CORPORATE SOURCE: Fac. Sci., Nagoya Univ., Nagoya, 464, Japan

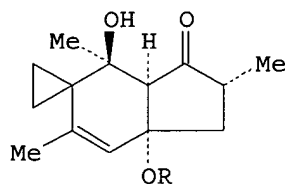
SOURCE: Tetrahedron Letters (1989), 30(15), 1983-6

CODEN: TELEAY; ISSN: 0040-4039

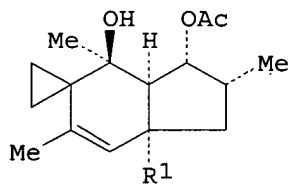
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

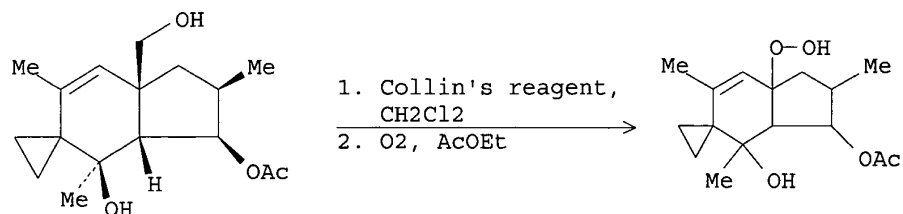


II

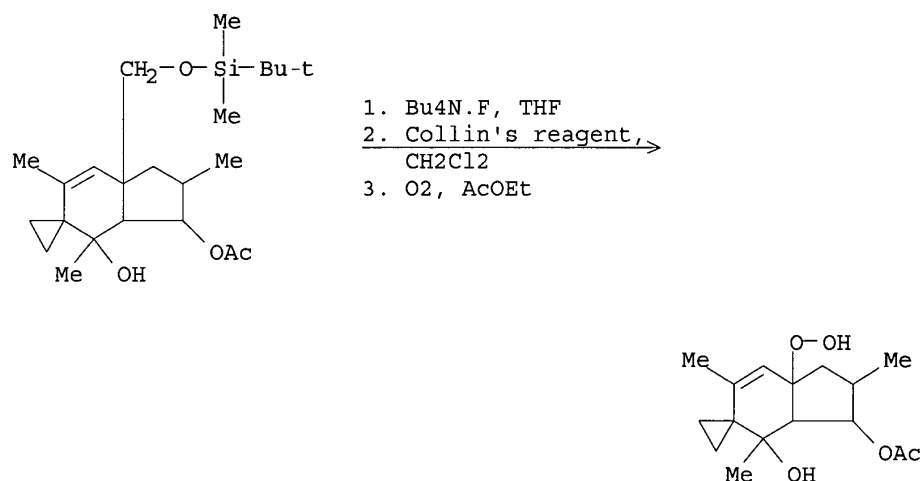
AB Starting from α-allyl-δ-valerolactone, a stereocontrolled synthesis of ptaquilosin (I; R = H), the aglycon of a bracken carcinogen ptaquiloside (I; R = glucosyl) was achieved in racemic form, which includes a novel deformylation-hydroxylation reaction via II (R1 = CHO,

OOH, OH) as one of the key steps.

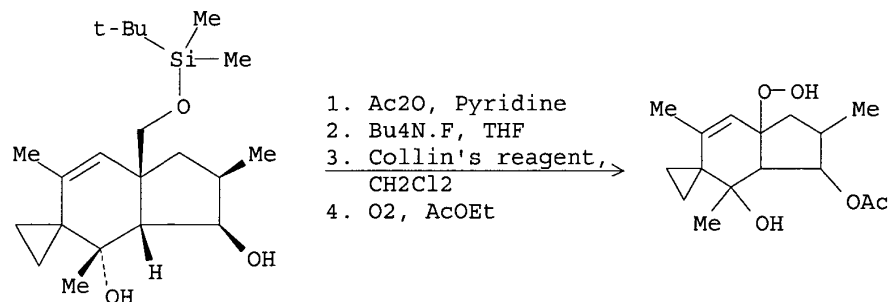
RX(59) OF 592 - 2 STEPS



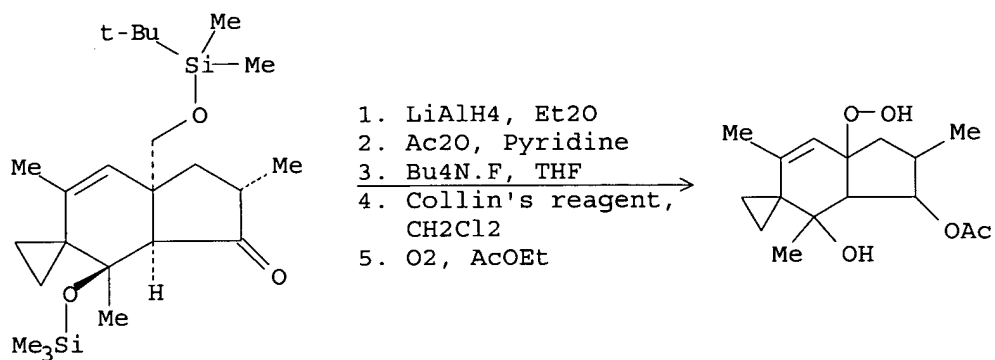
RX(142) OF 592 - 3 STEPS



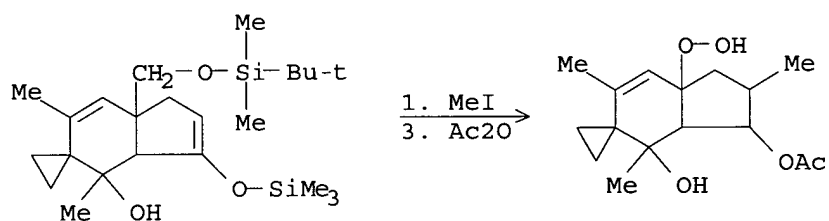
RX(143) OF 592 - 4 STEPS



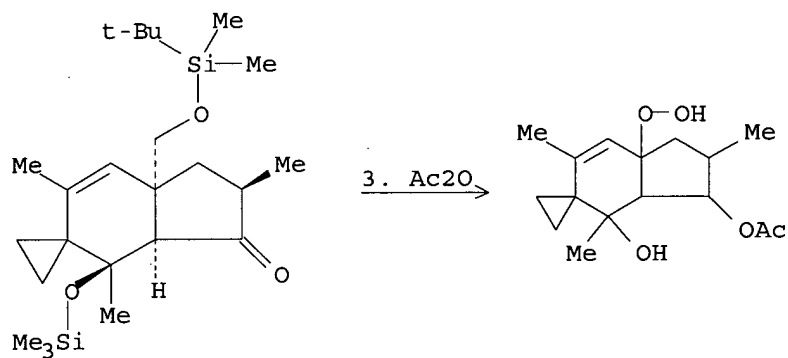
## RX(326) OF 592 - 5 STEPS



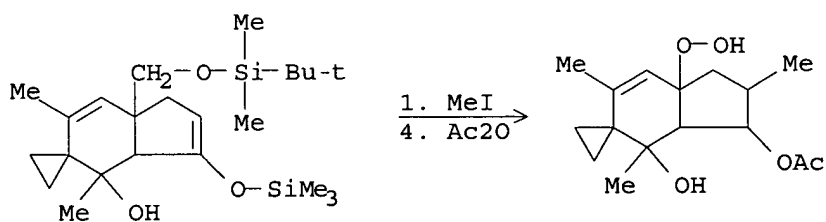
## RX(328) OF 592 - 6 STEPS



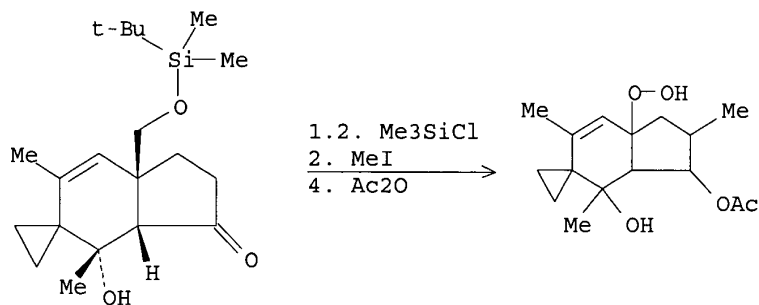
## RX(330) OF 592 - 6 STEPS



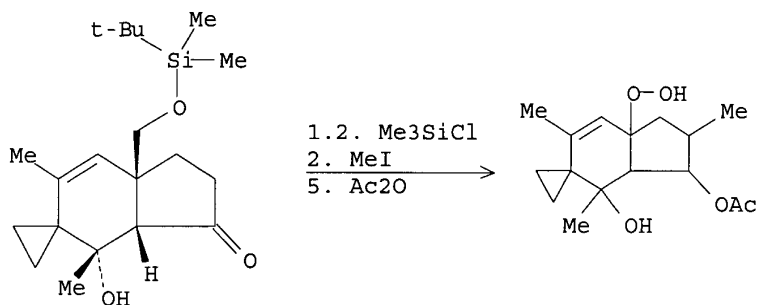
## RX(332) OF 592 - 7 STEPS



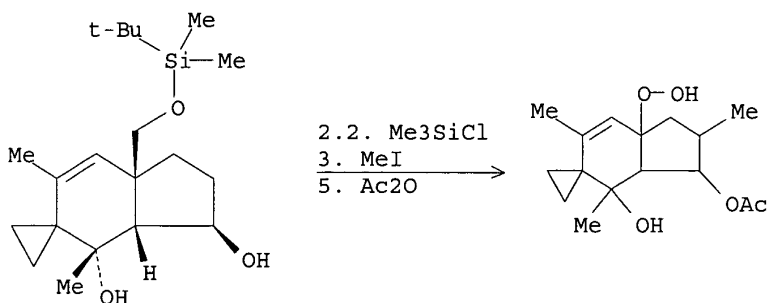
RX(334) OF 592 - 7 STEPS



RX(346) OF 592 - 8 STEPS

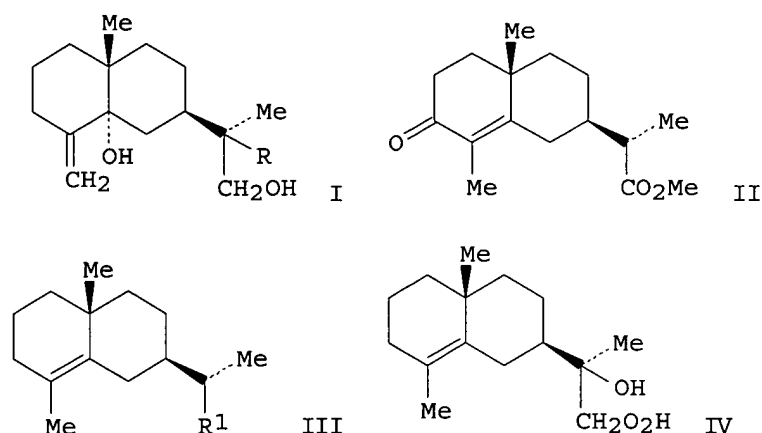


RX(347) OF 592 - 8 STEPS



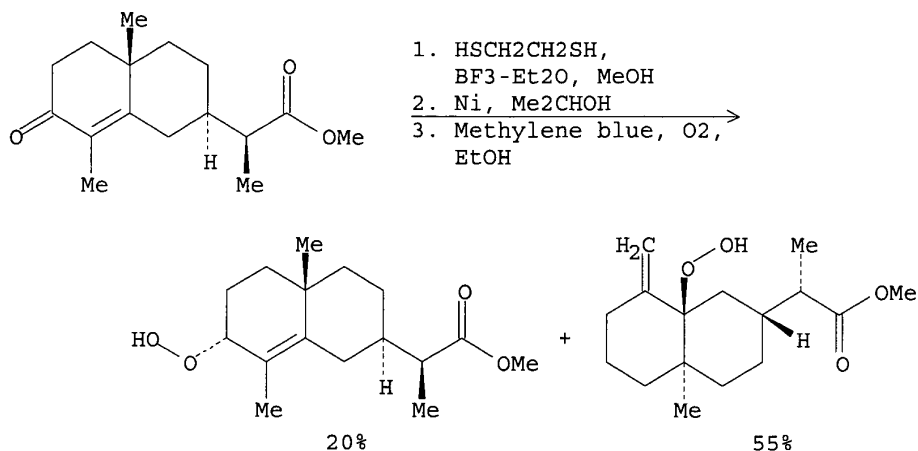
L34 ANSWER 16 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 111:115614 CASREACT  
TITLE: Approach to the synthesis of side-chain

eudesmanediols. Synthesis of kudtrial from  
 1-( $\alpha$ )-santonin  
 AUTHOR(S): Harapanhalli, Ravi S.  
 CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Bombay, 400 076,  
 India  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 1: Organic and Bio-Organic Chemistry (1972-1999)  
 (1988), (12), 3149-54  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



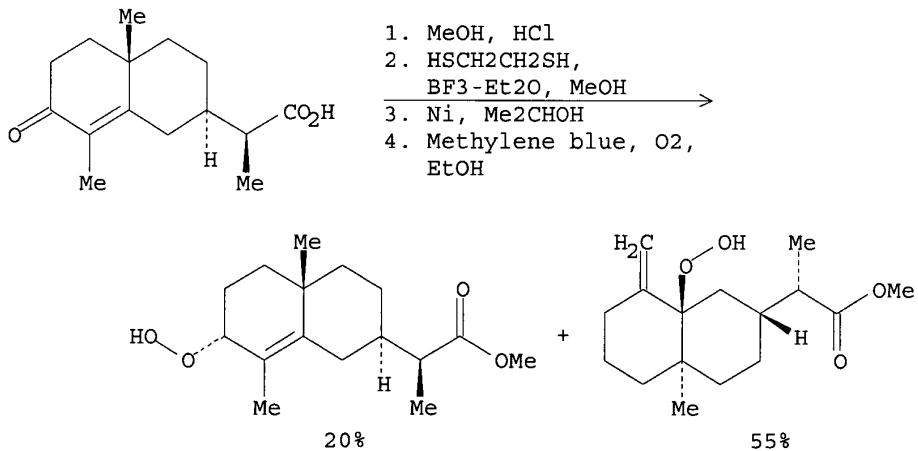
AB Kudtrial (I; R = OH) and its 11-deoxy analog I (R = H) were prepared from 1-( $\alpha$ )-santonin in ten steps. The known intermediate Me (11S)-3-oxoeudesm-4-en-12-oate (II) was taken through the new intermediates Me (11S)-eudesm-4-en-12-oate, (11S)-eudesm-4-en-12-al (III, R1 = CHO), 11-hydroxyeudesm-4-en-12-al, and eudesm-4-ene-11,12-diol (IV). The construction of side-chain diol moiety in IV was achieved by the application of Vedejs' enolate hydroxylation on III (R1 = CHO). The sensitized photooxygenation-reduction sequence transformed IV into I (R = OH). A similar sequence on (11S)-eudesm-4-en-12-ol (III; R1 = CH<sub>2</sub>OH) resulted in I (R = H).

## RX(39) OF 67 - 3 STEPS



NOTE: 3) photochem.

## RX(41) OF 67 - 4 STEPS

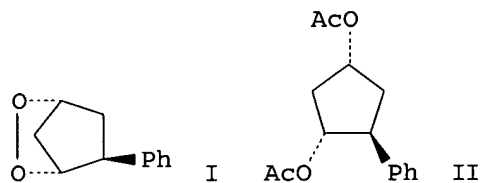


NOTE: 4) photochem.

L34 ANSWER 17 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 109:37642 CASREACT  
 TITLE: Formation of 1-phenyl-2,3-dioxabicyclo[2.2.1]heptane  
 in the reaction of 1,3-dibromo-4-phenylcyclopentane  
 with hydrogen peroxide in the presence of silver  
 trifluoroacetate  
 AUTHOR(S): Takahashi, Kimio; Shiro, Motoo; Kishi, Morio  
 CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka,  
 553, Japan  
 SOURCE: Journal of Organic Chemistry (1988), 53(13), 3098-104

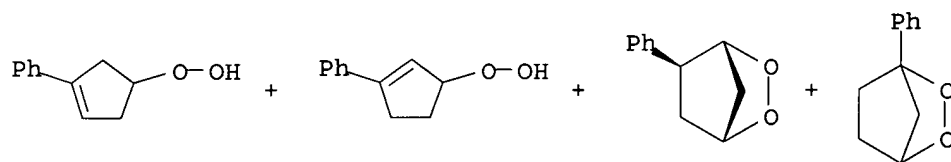
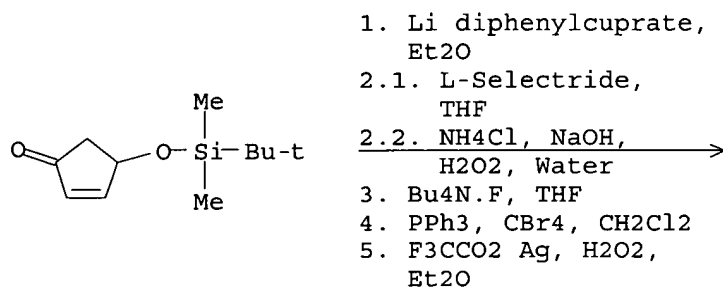
DOCUMENT TYPE:  
LANGUAGE:  
GI

CODEN: JOCEAH; ISSN: 0022-3263  
Journal  
English

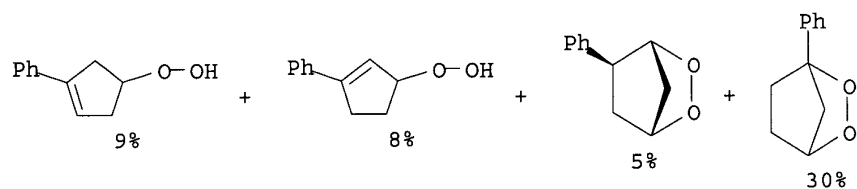
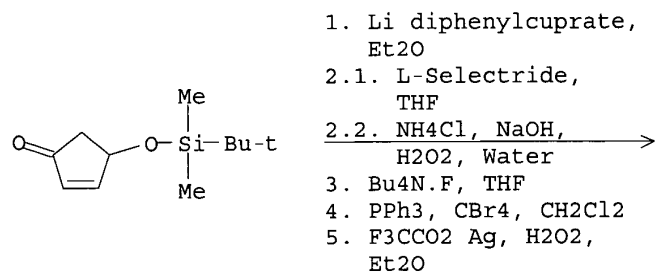


AB Reaction of 1,3-dibromo-4-phenylcyclopentane, prepared from 4-hydroxycyclopent-2-en-1-one in a stereocontrolled manner, or its stereoisomer with anhydrous  $\text{H}_2\text{O}_2$  in the presence of  $\text{CF}_3\text{CO}_2\text{Ag}$  gave 1-phenyl-2,3-dioxabicyclo[2.2.1]heptane as the main rearranged product. The expected 5-phenyl-2,3-dioxabicyclo[2.2.1]heptane (I) and phenylcyclopentenyl hydroperoxides were also formed in this reaction. An authentic sample of endoperoxide I was prepared by using peroxide transfer reaction between  $(\text{Bu}_3\text{SnO})_2$  and the bis(triflate) of all-cis-phenylcyclopentanediol. The stereochem. of I and related compds. was confirmed by correlation with the data from x-ray crystallog. anal. of the diacetate II obtained from I by  $\text{SnCl}_2$  reduction

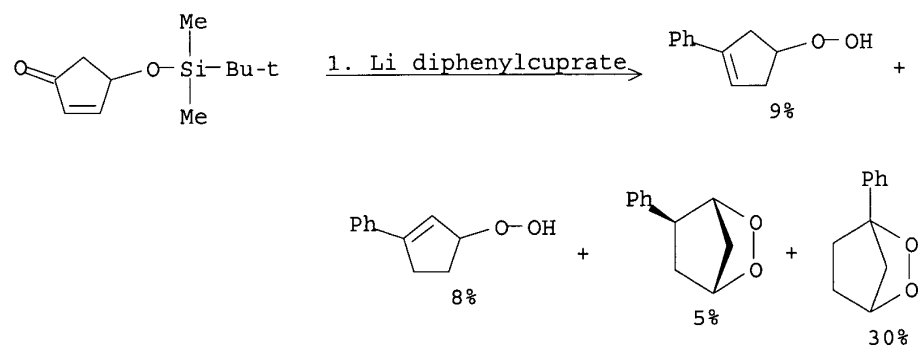
RX(179) OF 393 - 5 STEPS



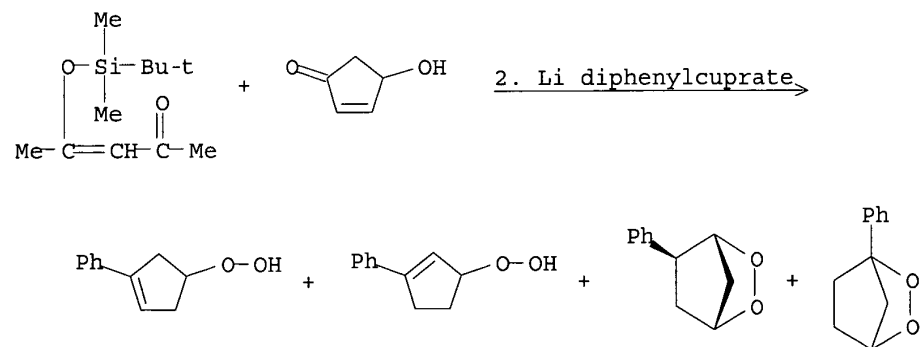
## RX(180) OF 393 - 5 STEPS



## RX(181) OF 393 - 5 STEPS

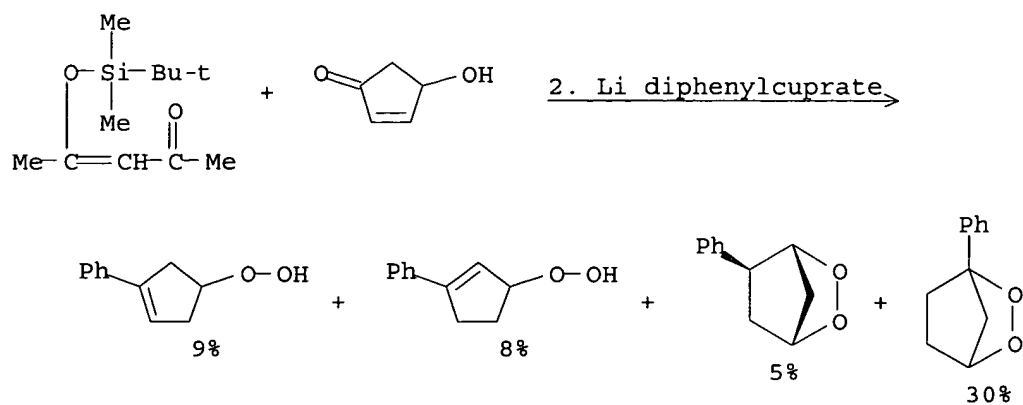


## RX(184) OF 393 - 6 STEPS

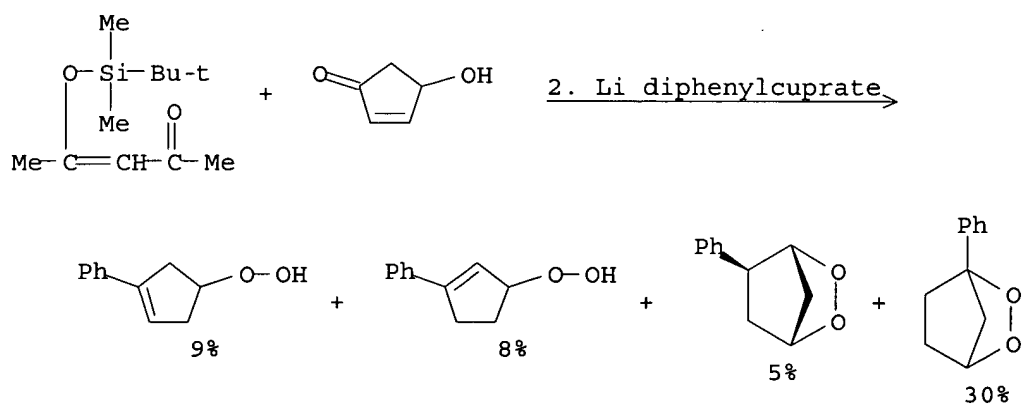




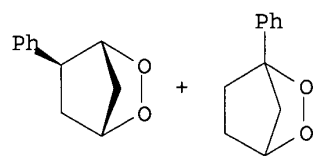
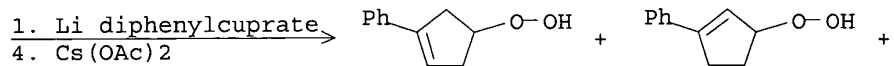
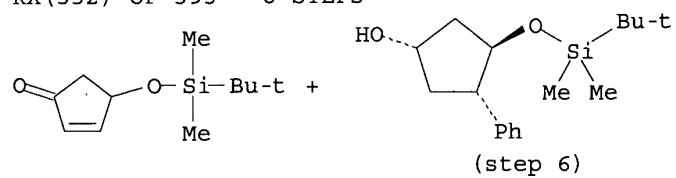
RX(185) OF 393 - 6 STEPS



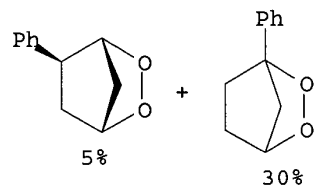
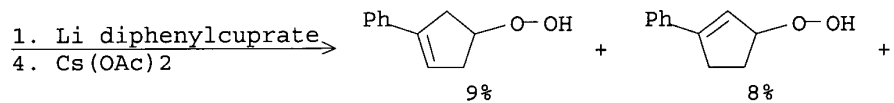
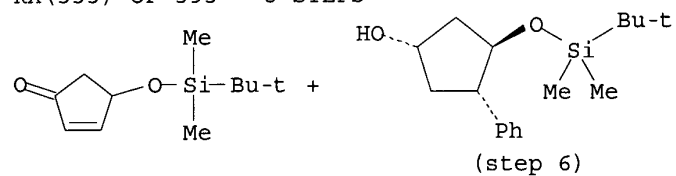
RX(186) OF 393 - 6 STEPS



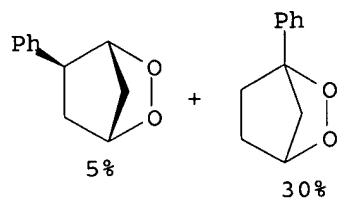
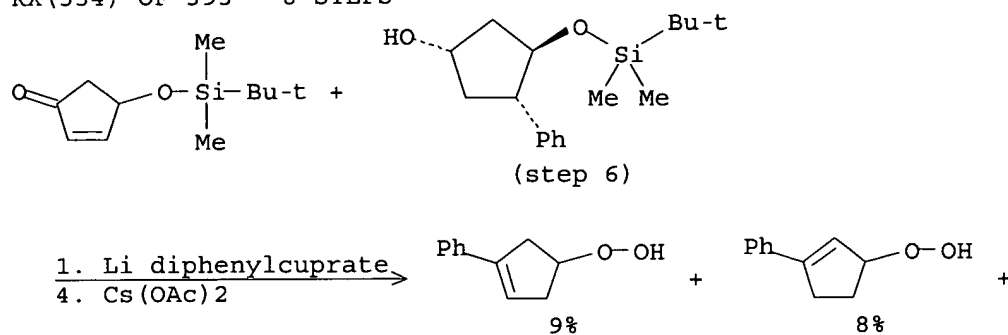
RX(332) OF 393 - 8 STEPS



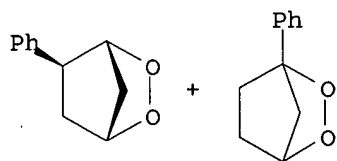
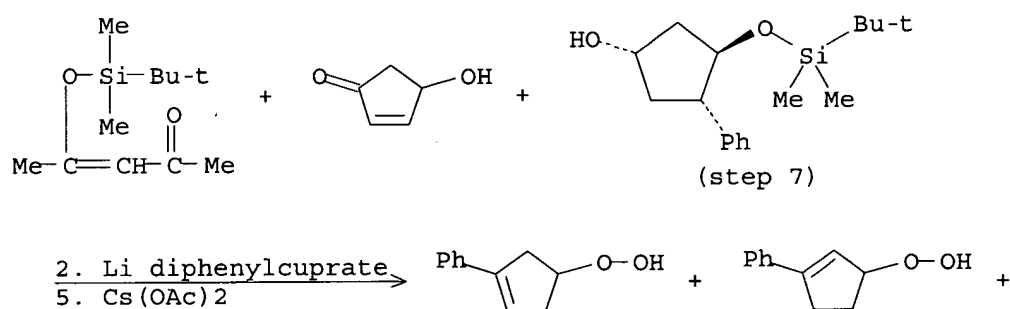
RX(333) OF 393 - 8 STEPS



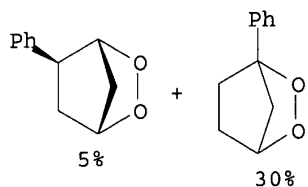
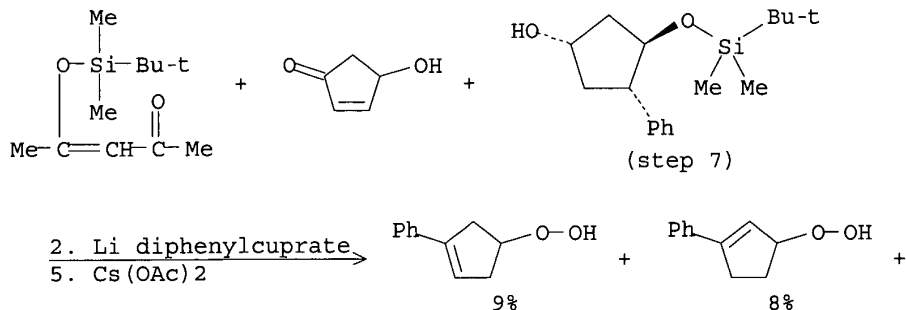
## RX(334) OF 393 - 8 STEPS



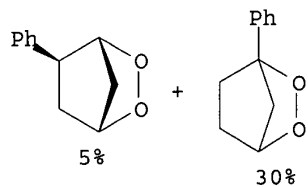
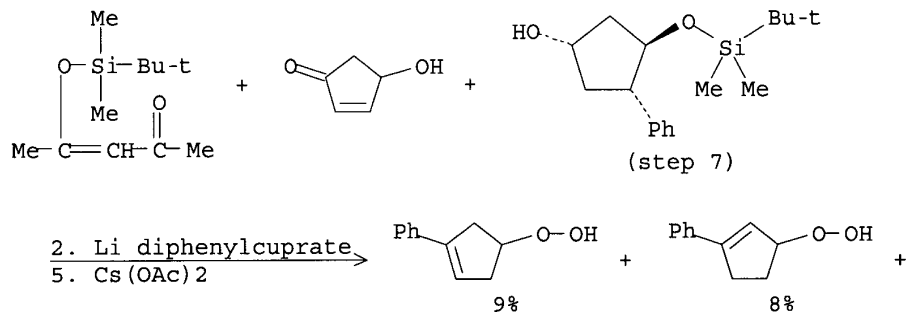
## RX(357) OF 393 - 9 STEPS



RX(358) OF 393 - 9 STEPS



RX(359) OF 393 - 9 STEPS



L34 ANSWER 18 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

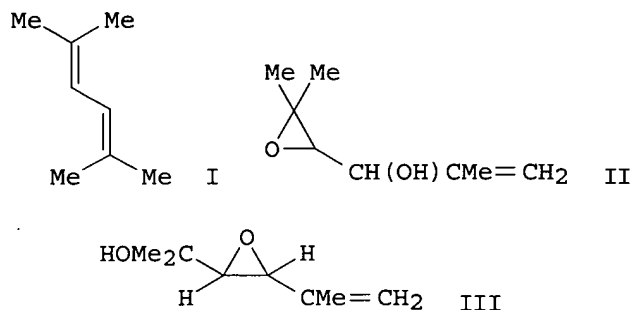
ACCESSION NUMBER:

109:6340 CASREACT

TITLE:

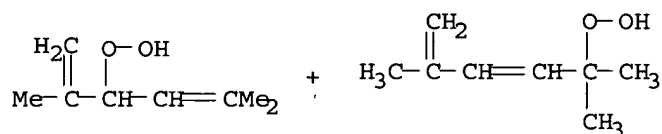
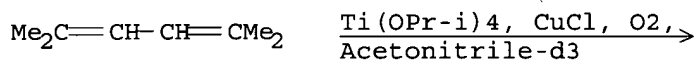
Regiocontrolled functionalization of  
 2,5-dimethyl-2,4-hexadiene into epoxy alcohols by  
 photooxygenation in the presence of titanium(IV) or

vanadium(V)  
 AUTHOR(S): Adam, Waldemar; Staab, Eugen  
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700,  
 Fed. Rep. Ger.  
 SOURCE: Tetrahedron Letters (1988), 29(5), 531-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Using  $\text{Ti}(\text{OCHMe}_2)_4$  as oxygen transfer catalyst, the diene I gave exclusively the epoxy alc. II, whereas the reaction with  $\text{VO}(\text{acac})_2$  gave exclusively the isomerized epoxy alc. III, via ene reaction with singlet oxygen.

RX(1) OF 16

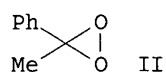


NOTE: singlet

L34 ANSWER 19 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 110:23463 CASREACT  
 TITLE: Oxygenation of nitroalkanes with cobalt Schiff base complexes  
 AUTHOR(S): Nishinaga, Akira; Morikawa, Shohei; Yoshida, Katsumi; Matsuura, Teruo  
 CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, 606, Japan  
 SOURCE: Nippon Kagaku Kaishi (1988), (4), 487-94  
 CODEN: NKAKB8; ISSN: 0369-4577  
 DOCUMENT TYPE: Journal

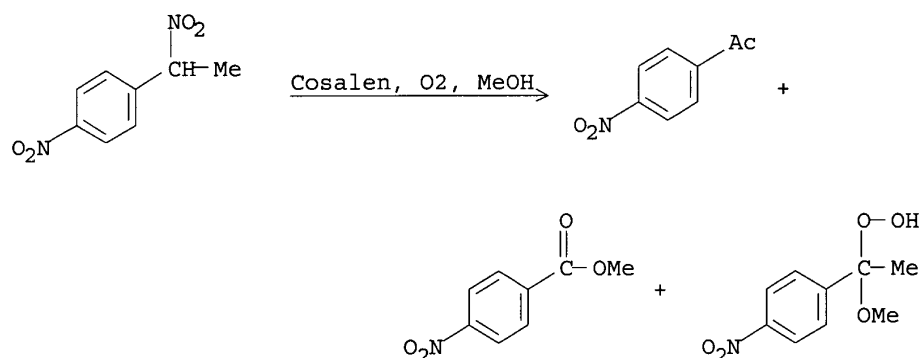
LANGUAGE:  
GI

Japanese



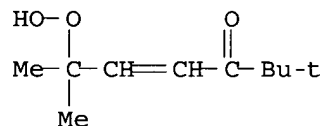
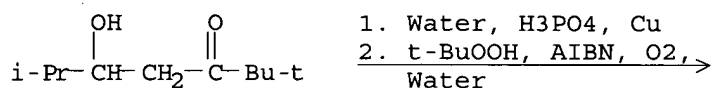
AB Cobalt Schiff base complexes promote the oxygenation of nitroalkanes to give corresponding carbonyl products and (ONO)CoIII(L) (L = Schiff base ligand). The highest selective formation of the carbonyl product with a high conversion is achieved by employing a coordinately saturated hydroxocobalt(III) complex. The oxygenation of PhCHMeNO<sub>2</sub> (I) with (HO)CoIII(salen) [salen = (2--OC<sub>6</sub>H<sub>4</sub>CH:NCH<sub>2</sub>)<sub>2</sub>], a coordinately unsatd. complex, in alcs. gave the corresponding substituted benzoic acid esters and PhAc. The reaction does not proceed catalytically, because the nitrocobalt(III) complex formed is inactive. Kinetic studies of the oxygenation of I show that the first step may be an acid-base equilibrium reaction between the substrate and the hydroxo complex giving a substrate anion cobalt(III) complex intermediate. Dioxygen is incorporated into the substrate anion species to give a (1-nitro-1-phenylethylperoxo)cobalt(III) complex, which may decompose to (ONO)CoIII(L) and the dioxirane II, and this dioxane further oxidizes the substrate or the substrate anion species selectively when the peroxocobalt(III) complex is coordinately saturated. Otherwise, the peroxo complex in alcs. ROH (R = Me, Et, Me<sub>2</sub>CH) decomps. to (ONO)CoIII(L) and PhCMe(OR)OOH, which undergoes the Baeyer-Villiger decomposition to the benzoic acid esters PhCO<sub>2</sub>R. A good evidence is available from the oxygenation of 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CHMeNO<sub>2</sub> with (HO)Co(salen) in MeOH, where 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CMe(OMe)OOH is isolated together with 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>Ac and 4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me.

RX(13) OF 15

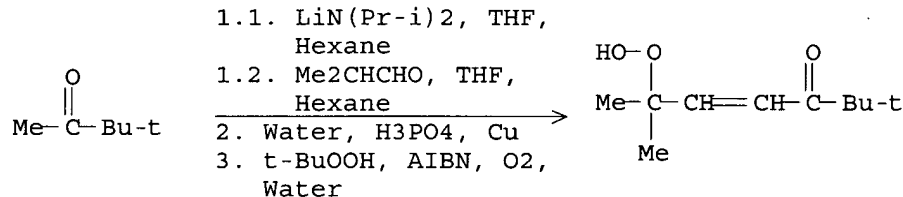


ACCESSION NUMBER: 110:38673 CASREACT  
 TITLE:  $\gamma$ -Hydroxylation of enones using tert-butyl hydroperoxide and oxygen  
 AUTHOR(S): Sabol, Mark R.; Wigglesworth, Charlene; Watt, David S.  
 CORPORATE SOURCE: Lucille Parker Markey Cancer Cent., Univ. Kentucky, Lexington, KY, 40506, USA  
 SOURCE: Synthetic Communications (1988), 18(1), 1-12  
 CODEN: SYNCAV; ISSN: 0039-7911  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Free radical hydroxylation of enones, e.g.  $\text{RCOCH:CHCHR}_1\text{R}_2$  [I; R = Me<sub>3</sub>C, R<sub>1</sub> = R<sub>2</sub> = Me, Et; R = PhMe<sub>2</sub>C, R<sub>1</sub> = R<sub>2</sub> = Me; R = PhMe<sub>2</sub>C, R<sub>1</sub>R<sub>2</sub> = (CH<sub>2</sub>)<sub>7</sub>] with Me<sub>3</sub>COOH-AIBN-O gave 28-68%  $\text{RCOCH:CHC(OH)R}_1\text{R}_2$  (II). The yields of II vary as a function of the substitution pattern of the  $\gamma$ -carbon of I. A homolytic mechanism is suggested in which Me<sub>3</sub>COOH serves as an initiator.

## RX(12) OF 14 - 2 STEPS

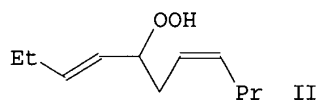


## RX(14) OF 14 - 3 STEPS



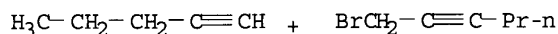
L34 ANSWER 21 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 109:92081 CASREACT  
 TITLE: Photosensitized oxidation of model unsaturated lipid systems: (4Z,7Z)-undeca-4,7-diene and (4Z)-undec-4-en-7-yne  
 AUTHOR(S): Carless, Howard A. J.; Batten, Richard J.  
 CORPORATE SOURCE: Dep. Chem., Birkbeck Coll., London, WC1E 7HX, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (9), 1999-2007  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

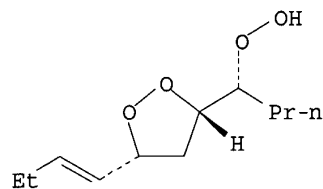
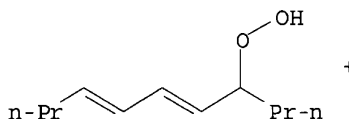


AB The photosensitized oxidation of the skipped diene (4Z,7Z)-4,7-undecadiene (I) gave hydroperoxides II and III in a 2:3 ratio. Free radical cyclization of II gave the stereoisomeric dioxolanyl hydroperoxides IV. (4Z)-4-Undecen-7-yne (V) on photosensitized oxidation gave a 1:2 mixture of the nonconjugated and conjugated enynyl hydroperoxides VI and VII. 4,7-Undecadiyne (VIII) was comparatively resistant to photosensitized oxidation; the relative rates of attack on I, V, and VIII are 110:15:≤1. There was no evidence for the abstraction of the 2-propynyl hydrogen by singlet oxygen.

RX(36) OF 65 - 4 STEPS



- 1.1. EtMgBr, THF
- 1.2. PBr<sub>3</sub>, CuCl, THF
- 1.3. THF
2. H<sub>2</sub>, MeOH
3. Tetraphenylporphine,  
O<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>
4. O<sub>2</sub>, (t-BuO<sub>3</sub>C)<sub>2</sub>,  
CCl<sub>4</sub>

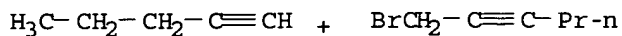


stereoisomers

NOTE: 2) Lindlar catalyst, 3) Photochem.



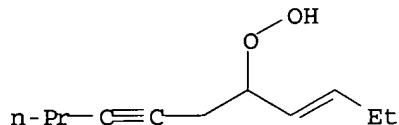
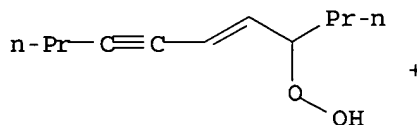
RX(43) OF 65 - 3 STEPS



- 1.1. EtMgBr, THF
- 1.2. PBr3, CuCl, THF
- 1.3. THF

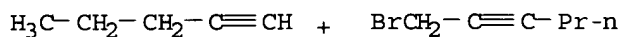
2. H2, MeOH

3. Tetraphenylporphine,  
O2, CH2Cl2



NOTE: 2) Lindlar catalyst, 3) Photochem.

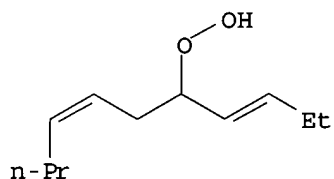
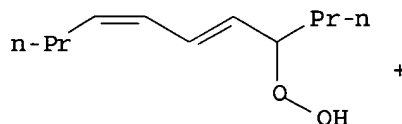
RX(44) OF 65 - 3 STEPS



- 1.1. EtMgBr, THF
- 1.2. PBr3, CuCl, THF
- 1.3. THF

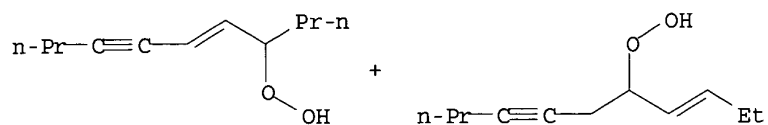
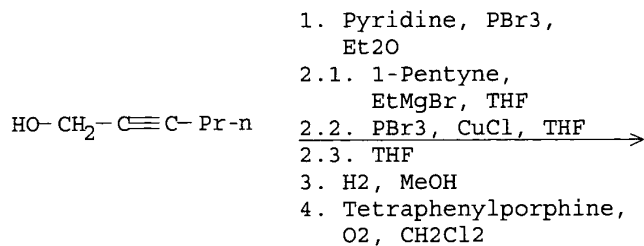
2. H2, MeOH

3. Tetraphenylporphine,  
O2, CH2Cl2



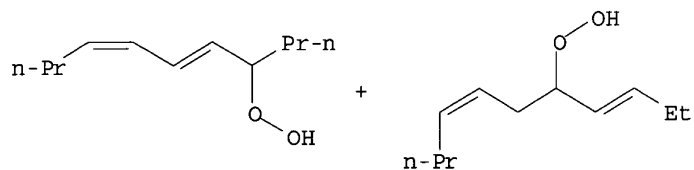
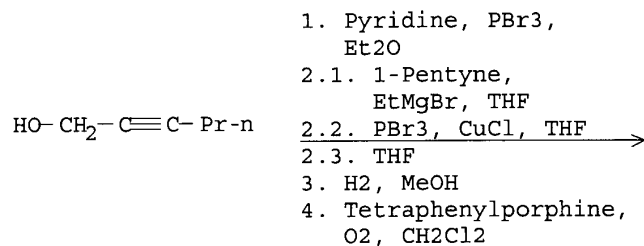
NOTE: 2) Lindlar catalyst, 3) Photochem.

RX(45) OF 65 - 4 STEPS



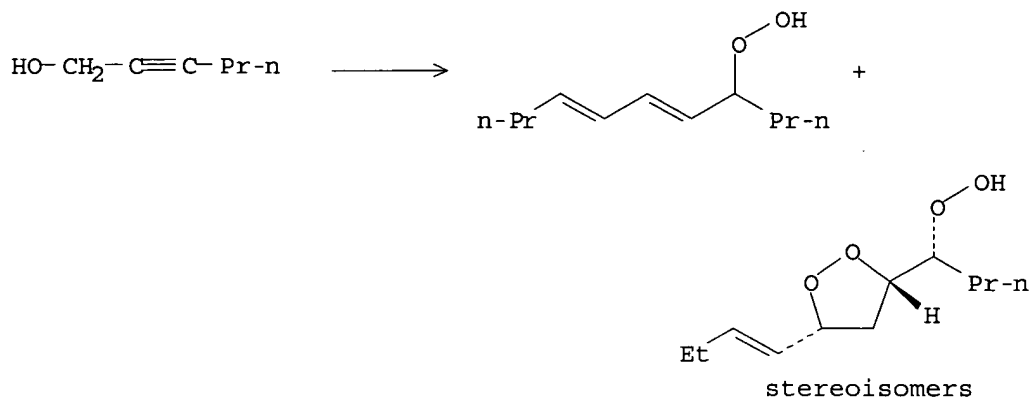
NOTE: 3) Lindlar catalyst, 4) Photochem.

RX(46) OF 65 - 4 STEPS



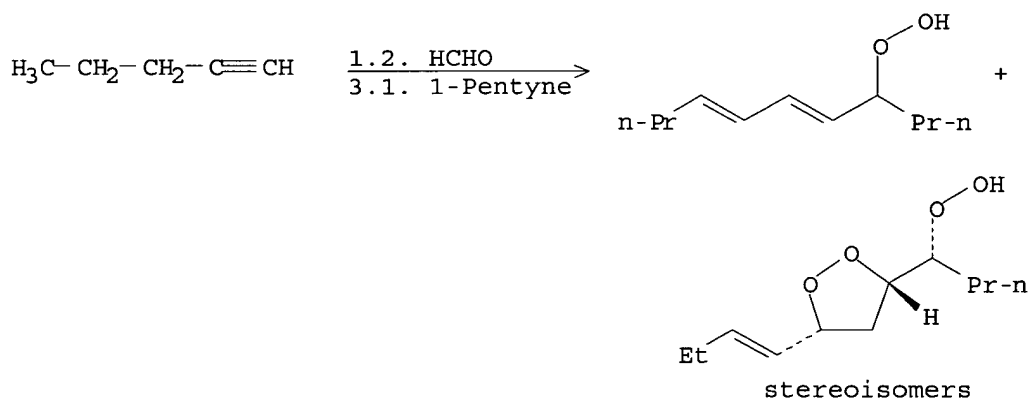
NOTE: 3) Lindlar catalyst, 4) Photochem.

RX(50) OF 65 - 5 STEPS



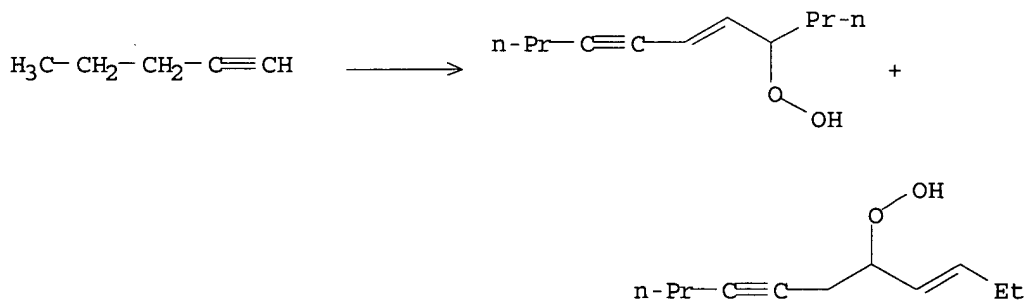
NOTE: 3) Lindlar catalyst, 4) Photochem.

RX(54) OF 65 - 6 STEPS



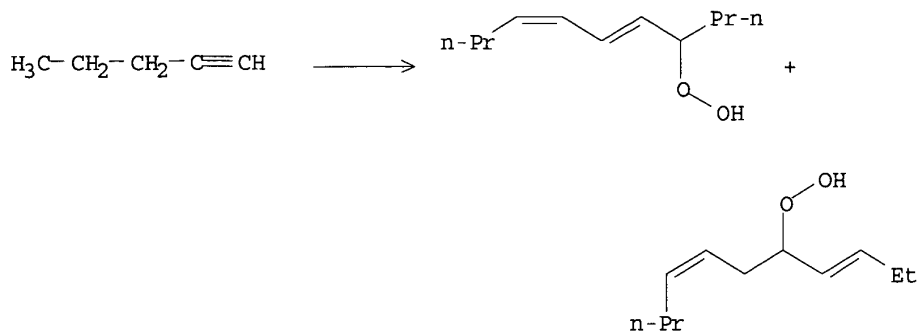
NOTE: 1) PARAFORMALDEHYDE USED, 4) Lindlar catalyst, 5) Photochem.

RX(55) OF 65 - 5 STEPS



NOTE: 1) PARAFORMALDEHYDE USED, 4) Lindlar catalyst, 5) Photochem.

RX(56) OF 65 - 5 STEPS



NOTE: 1) PARAFORMALDEHYDE USED, 4) Lindlar catalyst, 5) Photochem.

L34 ANSWER 22 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

106:5257 CASREACT

TITLE:

Practical conversion of artemisinin acid in desoxyartemisinin

AUTHOR(S):

Jung, Mankil; ElSohly, Hala N.; Croom, Edward M.; McPhail, Andrew T.; McPhail, Donald R.

CORPORATE SOURCE:

Sch. Pharm., Univ. Mississippi, University, MS, 38677, USA

SOURCE:

Journal of Organic Chemistry (1986), 51(26), 5417-19  
CODEN: JOCEAH; ISSN: 0022-3263

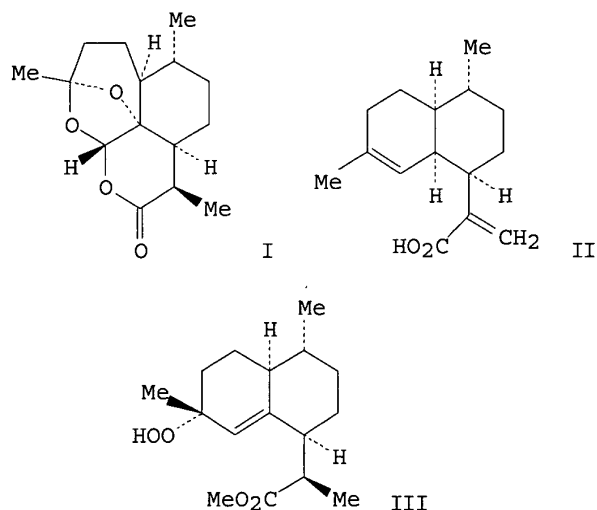
DOCUMENT TYPE:

Journal

LANGUAGE:

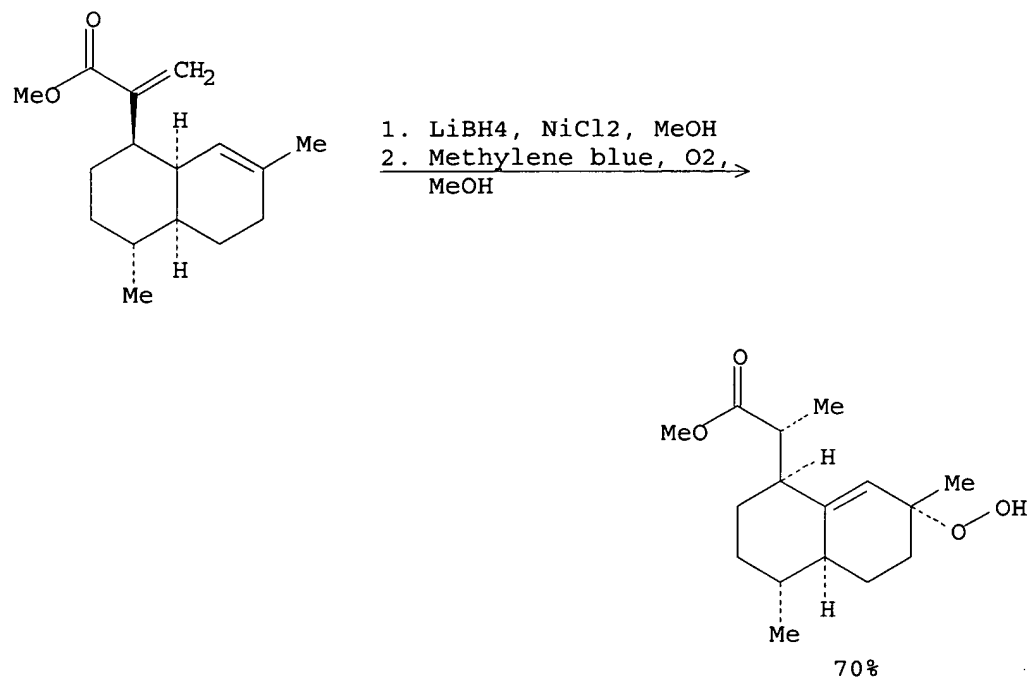
English

GI

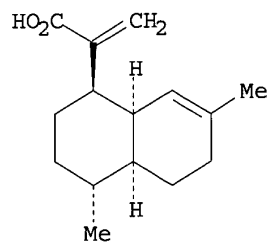


AB Deoxyartemisinin (I) was prepared from artemisinic acid (II) via allylic hydroperoxide III. The structure and absolute configuration of I were confirmed by x-ray crystallog.

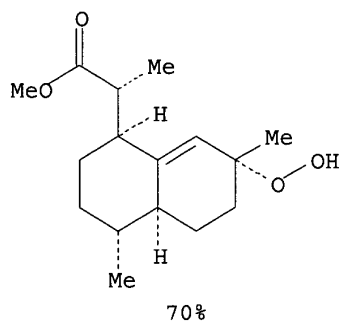
RX(7) OF 11 - 2 STEPS



RX(9) OF 11 - 3 STEPS



1. CH<sub>2</sub>N<sub>2</sub>, Et<sub>2</sub>O
2. LiBH<sub>4</sub>, NiCl<sub>2</sub>, MeOH
3. Methylene blue, O<sub>2</sub>, MeOH



L34 ANSWER 23 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

107:23517 CASREACT

TITLE:

Total syntheses of rothin-A and rothin-B

AUTHOR(S):

Carda, Miguel; Arno, Manuel; Marco, J. Alberto

CORPORATE SOURCE:

Dep. Quim. Org., Fac. Quim., Valencia, Spain

SOURCE:

Tetrahedron (1986), 42(13), 3655-62

CODEN: TETRAB; ISSN: 0040-4020

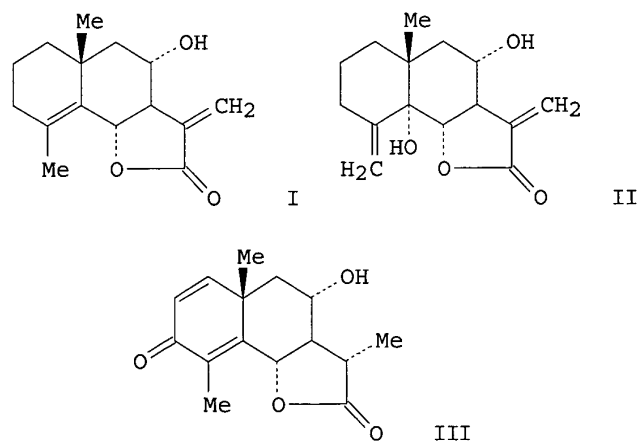
DOCUMENT TYPE:

Journal

LANGUAGE:

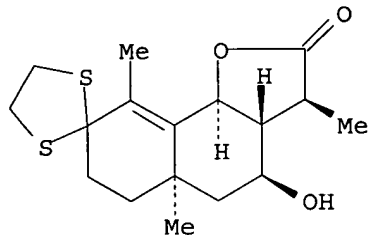
English

GI

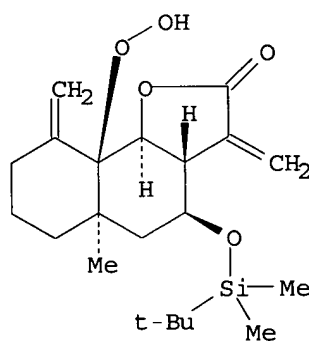


AB The eudesmanolides rothin A (I) and rothin B (II) have been synthesized from (-)-artemisin (III) in 7 and 9 steps, resp.

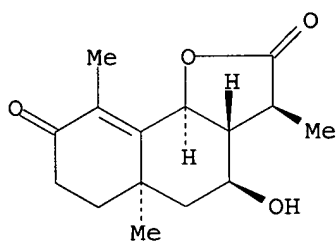
RX(63) OF 99 - 5 STEPS



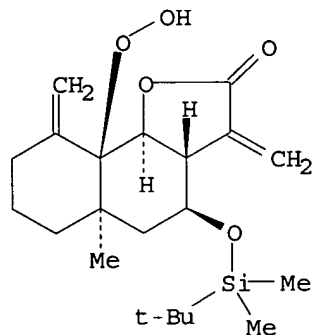
1. Ni
2.  $t\text{-BuSiMe}_2\text{Cl}$ ,  
1H-Imidazole, DMF
3.  $\text{PhSeCl}$ ,  $\text{LiN}(\text{Pr-}i)_2$ ,  
Hexane
4.  $\text{H}_2\text{O}_2$ , AcOH
5. Methylene blue,  
EtOH



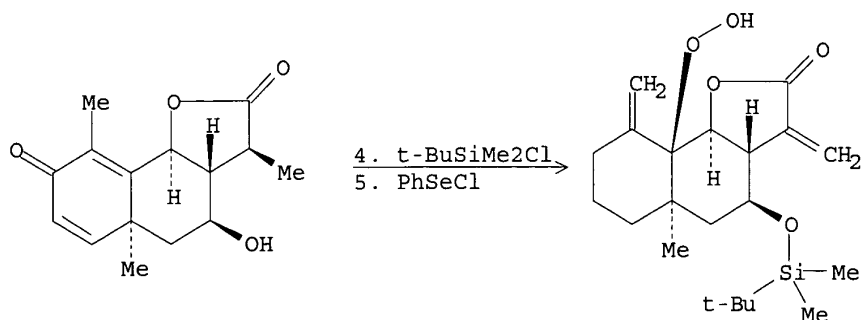
RX(70) OF 99 - 6 STEPS



3.  $t\text{-BuSiMe}_2\text{Cl}$
4.  $\text{PhSeCl}$



RX(77) OF 99 - 7 STEPS



L34 ANSWER 24 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 105:114794 CASREACT

TITLE: Synthesis of polyether-type tetrahydrofurans via hydroperoxide cyclization

AUTHOR(S): Bartlett, Paul A.; Chapuis, Christian

CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA

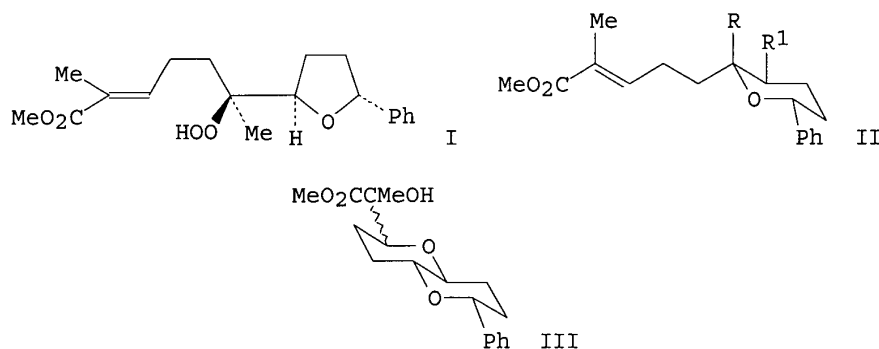
SOURCE: Journal of Organic Chemistry (1986), 51(14), 2799-806

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

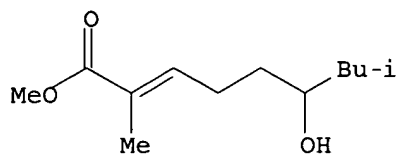


AB Isomerization of an unsatd. hydroperoxy ester to the epoxy alc. and then to the THF was investigated as a method for the stereocontrolled construction of ethers with a substitution pattern appropriate for polyether synthesis. This sequence is highly stereoselective in the case of secondary hydroperoxides, such as  $\text{MeO}_2\text{CCMe:CHCH}_2\text{CH}_2\text{CHPhOOH}$ , both with respect to the THF stereochem. and the acyclic relationship. With tertiary hydroperoxides, such as  $\text{MeO}_2\text{CCMe:CHCH}_2\text{CH}_2\text{CRMeOOH}$  ( $\text{R} = \text{Ph}$ ,  $\text{CH}_2\text{CHMe}_2$ ), little stereocontrol is seen over the ring stereochem. In the case of the hydroperoxide I, for example, the trans,cis and trans,trans bis ethers are formed in a 1.4:1 ratio. I was prepared stereospecifically from the pyran II ( $\text{R} = \text{Me}$ ,  $\text{R} = \text{Br}$ ) by a ring contraction process; however,

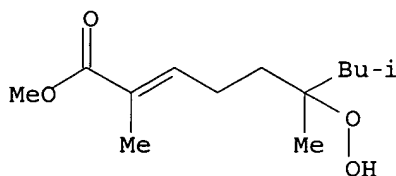


when this method was applied to II (R = H, R1 = iodo), II (R = H, R1 = OOH) was the major product. Cyclization of II (R = H, R1 = OOH) gave a mixture of the fused bis ethers III.

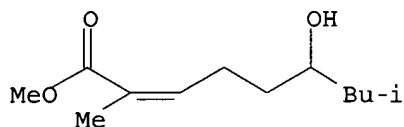
## RX(205) OF 707 - 4 STEPS



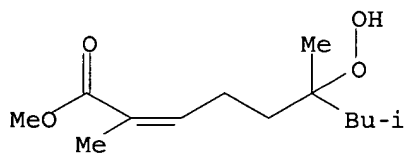
1. PCC, CH<sub>2</sub>Cl<sub>2</sub>
2. MeLi, THF
3. PPh<sub>3</sub>, CBr<sub>4</sub>,  
Benzene
4. F<sub>3</sub>CCO<sub>2</sub> Ag, H<sub>2</sub>O<sub>2</sub>,  
THF



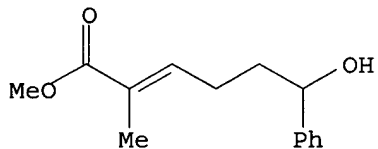
## RX(227) OF 707 - 4 STEPS



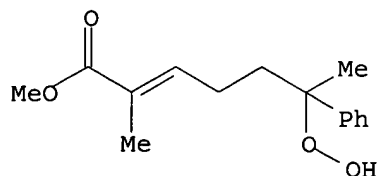
1. PCC, CH<sub>2</sub>Cl<sub>2</sub>
2. MeLi, THF
3. PPh<sub>3</sub>, CBr<sub>4</sub>,  
Benzene
4. F<sub>3</sub>CCO<sub>2</sub> Ag, H<sub>2</sub>O<sub>2</sub>,  
THF



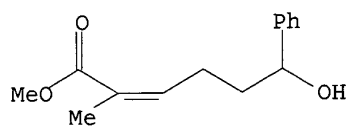
## RX(280) OF 707 - 4 STEPS



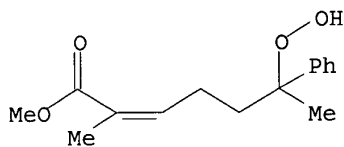
1. PCC, CH<sub>2</sub>Cl<sub>2</sub>
2. MeLi, THF
3. Me<sub>3</sub>SiBr, CH<sub>2</sub>Cl<sub>2</sub>
4. F<sub>3</sub>CCO<sub>2</sub> Ag, H<sub>2</sub>O<sub>2</sub>,  
THF



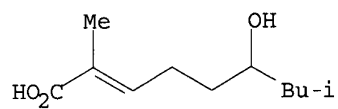
RX(288) OF 707 - 4 STEPS



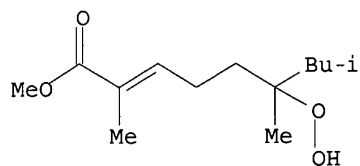
1. PCC, CH<sub>2</sub>Cl<sub>2</sub>
2. MeLi, THF
3. Me<sub>3</sub>SiBr, CH<sub>2</sub>Cl<sub>2</sub>
4. F<sub>3</sub>CCO<sub>2</sub> Ag, H<sub>2</sub>O<sub>2</sub>, THF



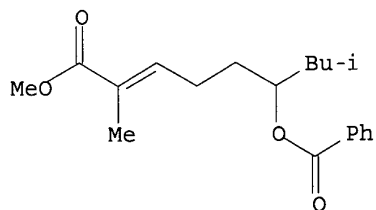
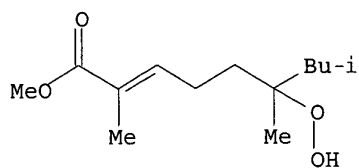
RX(358) OF 707 - 5 STEPS



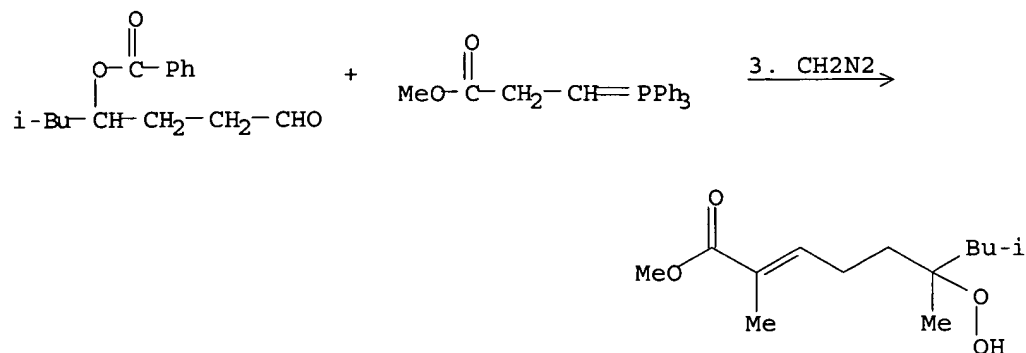
1. CH<sub>2</sub>N<sub>2</sub>, Et<sub>2</sub>O
2. PCC, CH<sub>2</sub>Cl<sub>2</sub>
3. MeLi, THF
4. PPh<sub>3</sub>, CBr<sub>4</sub>, Benzene
5. F<sub>3</sub>CCO<sub>2</sub> Ag, H<sub>2</sub>O<sub>2</sub>, THF



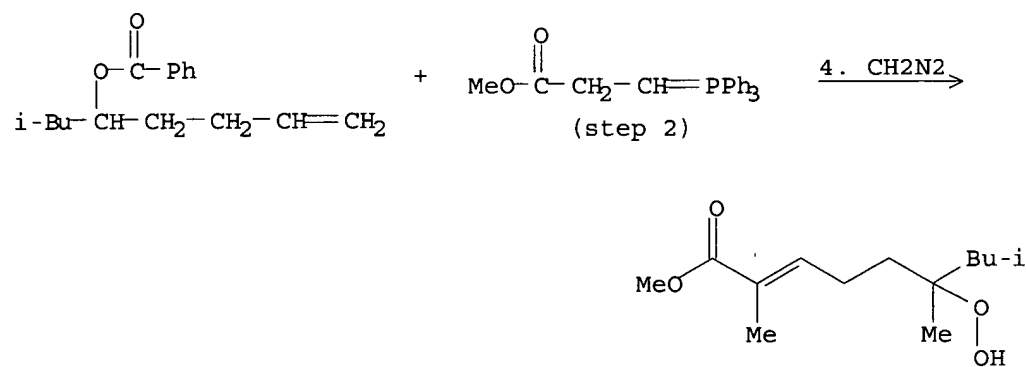
RX(360) OF 707 - 6 STEPS

2. CH<sub>2</sub>N<sub>2</sub> →

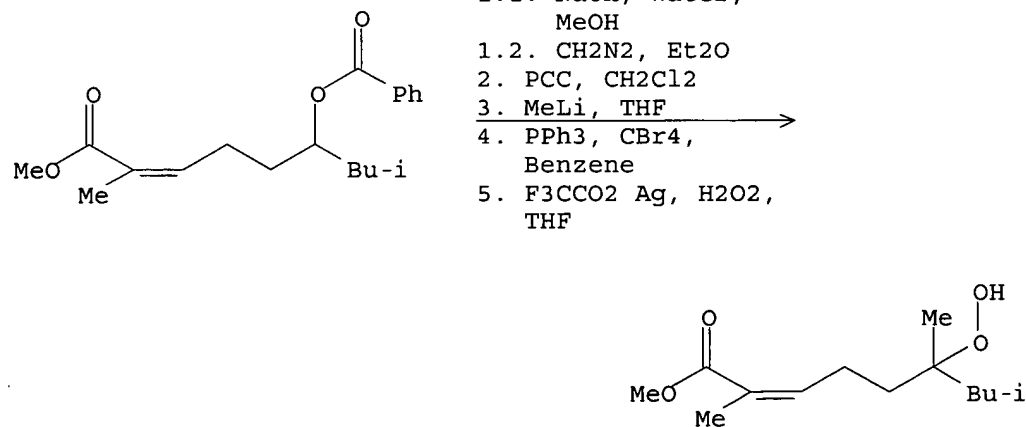
RX(362) OF 707 - 7 STEPS



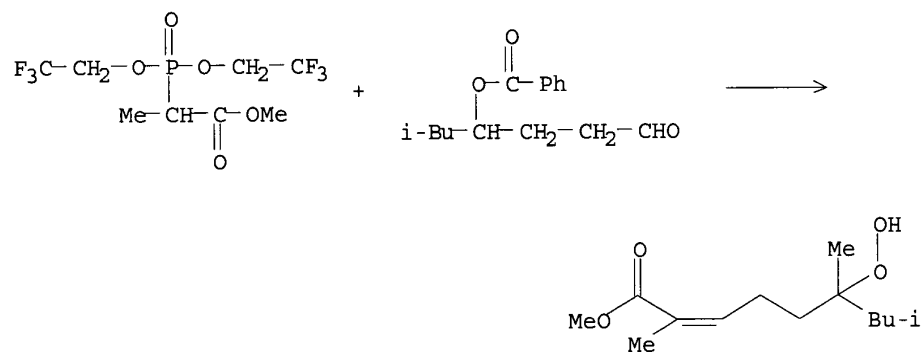
RX(364) OF 707 - 8 STEPS



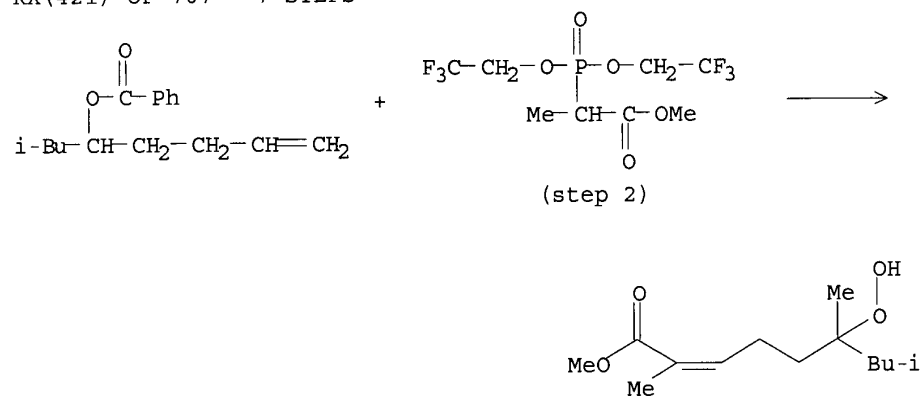
RX(417) OF 707 - 5 STEPS



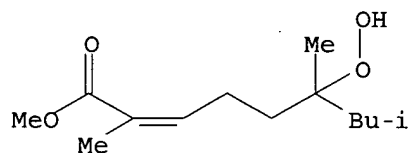
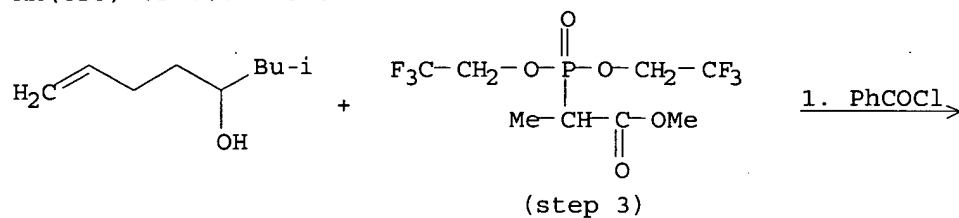
RX(419) OF 707 - 6 STEPS



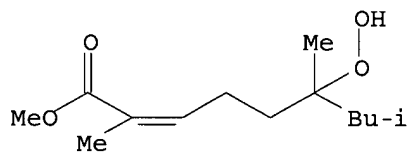
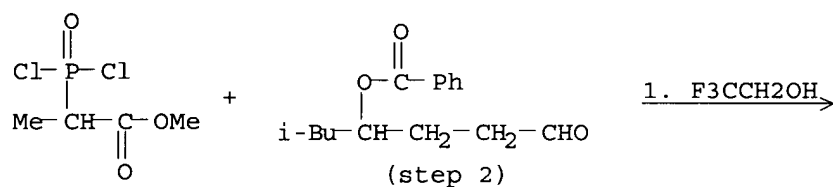
RX(421) OF 707 - 7 STEPS



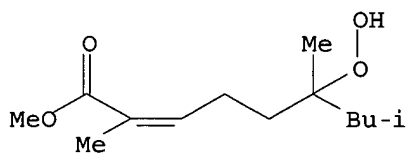
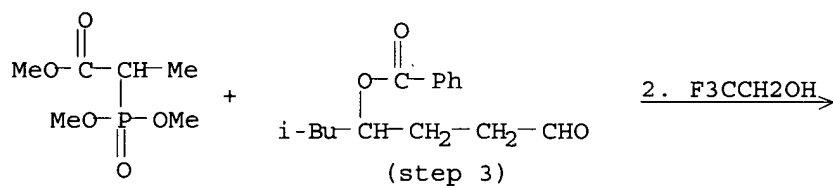
## RX(423) OF 707 - 8 STEPS



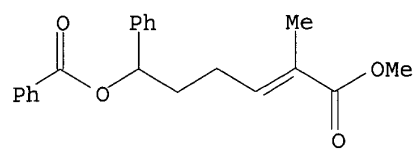
## RX(425) OF 707 - 7 STEPS



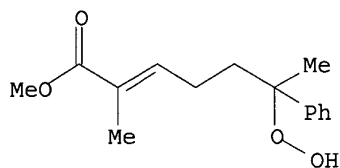
## RX(427) OF 707 - 8 STEPS



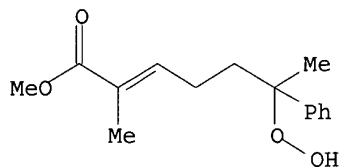
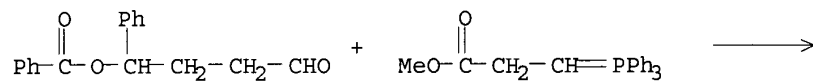
RX(498) OF 707 - 5 STEPS



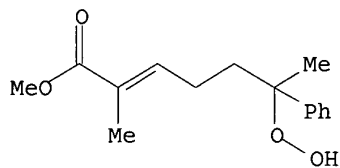
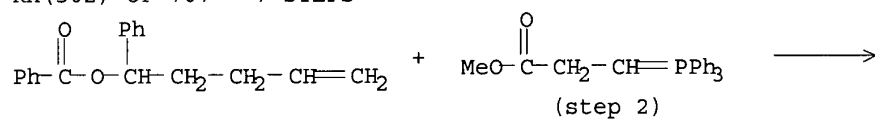
1. NaOH, Water, MeOH
2. PCC, CH<sub>2</sub>Cl<sub>2</sub>
3. MeLi, THF
4. Me<sub>3</sub>SiBr, CH<sub>2</sub>Cl<sub>2</sub>
5. F<sub>3</sub>CCO<sub>2</sub> Ag, H<sub>2</sub>O<sub>2</sub>, THF



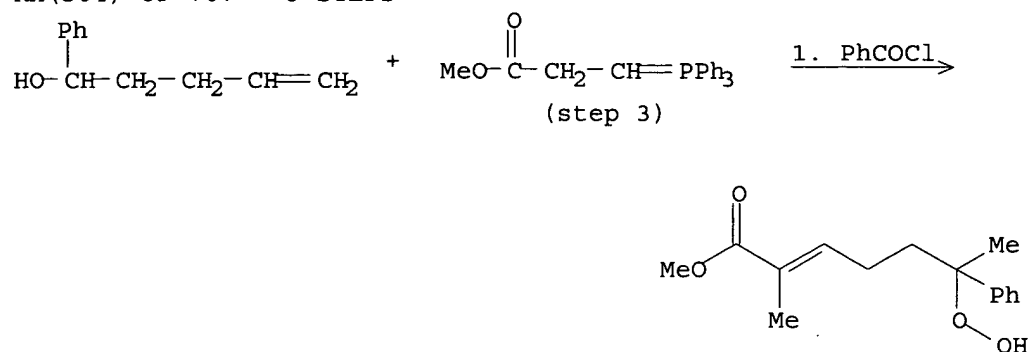
RX(500) OF 707 - 6 STEPS



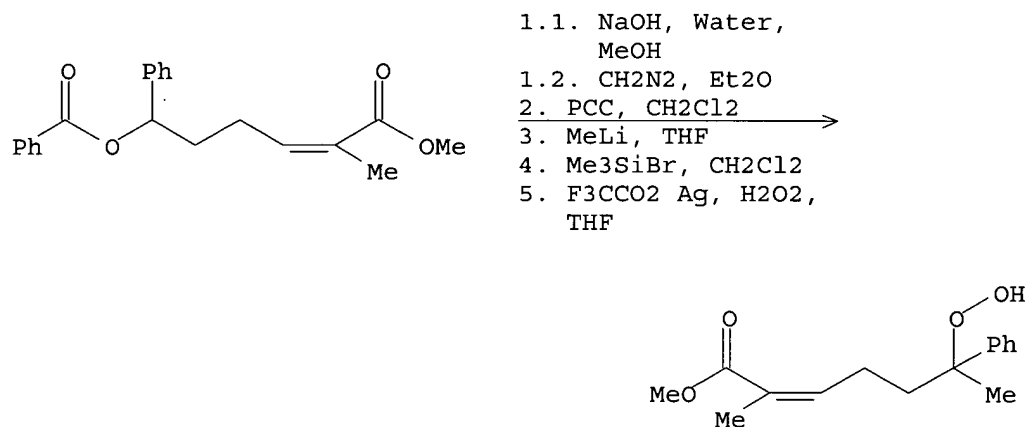
RX(502) OF 707 - 7 STEPS



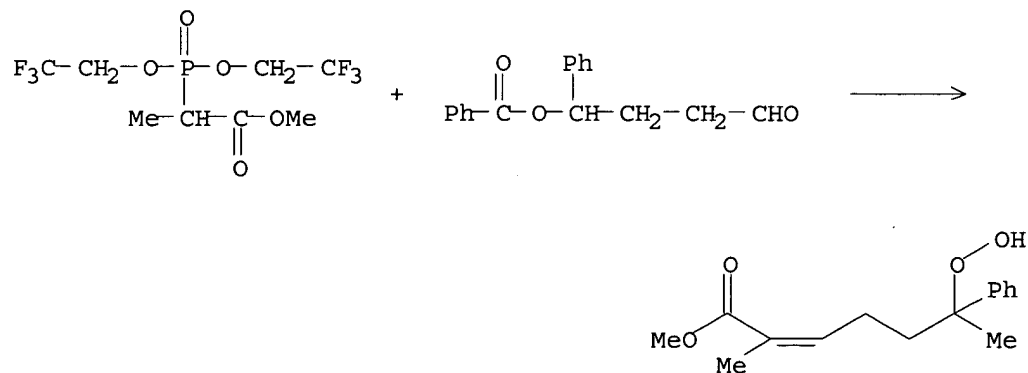
RX(504) OF 707 - 8 STEPS



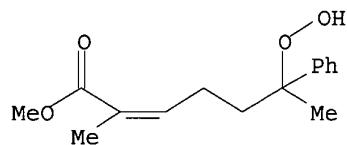
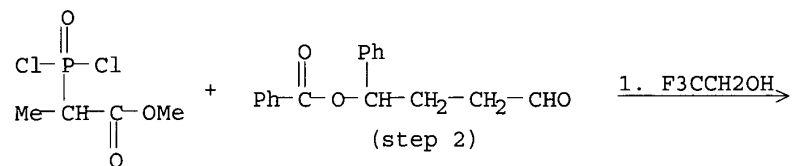
RX(542) OF 707 - 5 STEPS



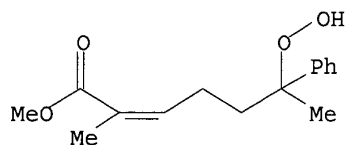
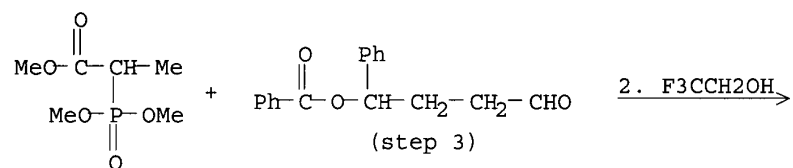
RX(544) OF 707 - 6 STEPS



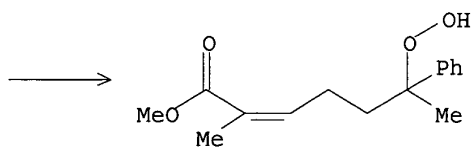
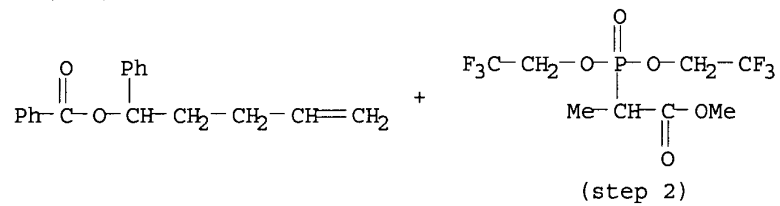
RX(546) OF 707 - 7 STEPS



RX(548) OF 707 - 8 STEPS

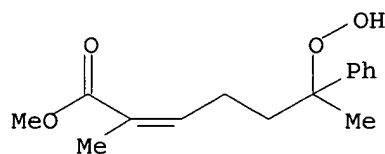
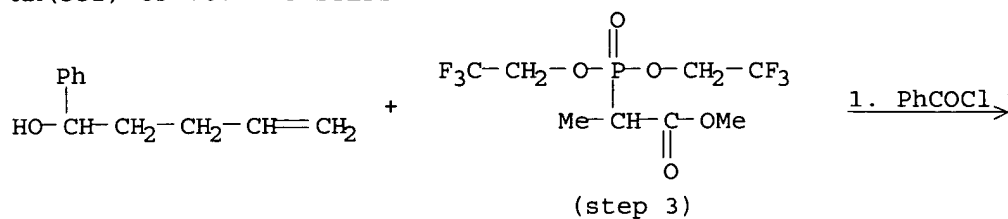


RX(550) OF 707 - 7 STEPS

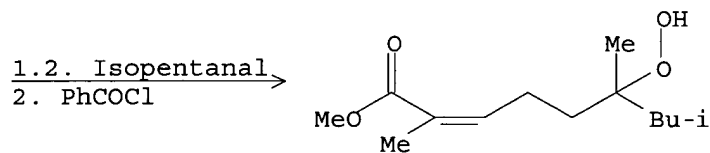
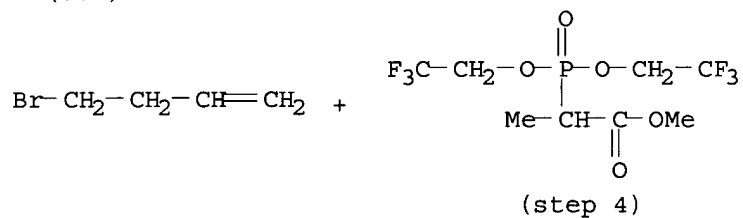




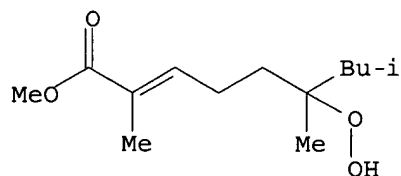
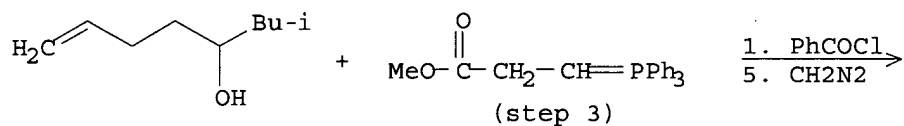
RX(552) OF 707 - 8 STEPS



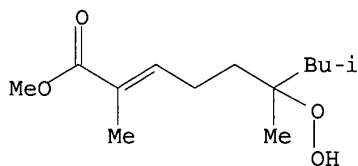
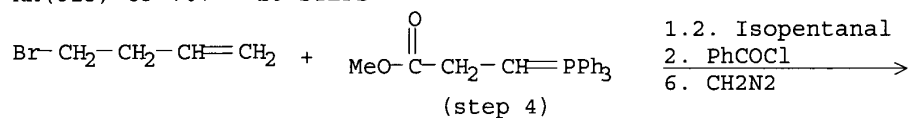
RX(604) OF 707 - 9 STEPS



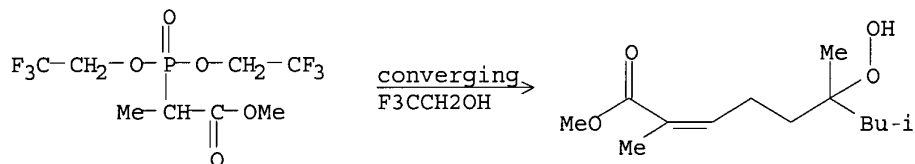
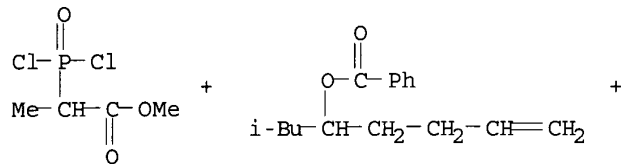
RX(606) OF 707 - 9 STEPS



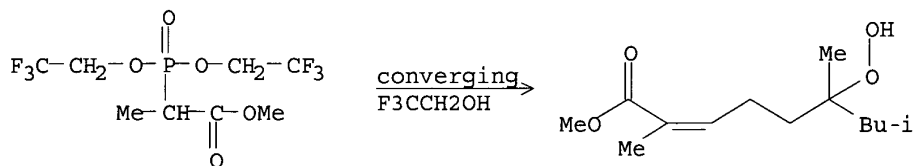
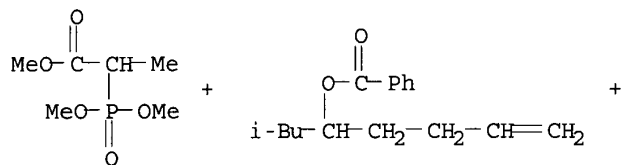
RX(613) OF 707 - 10 STEPS



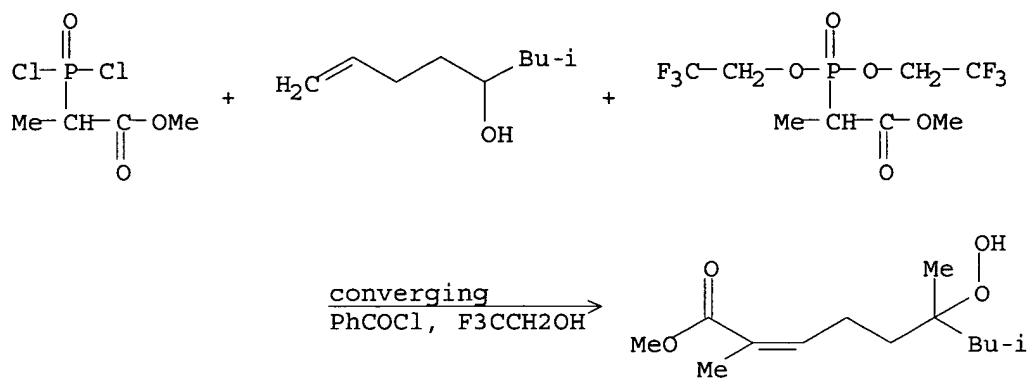
RX(621) OF 707 - 8 STEPS



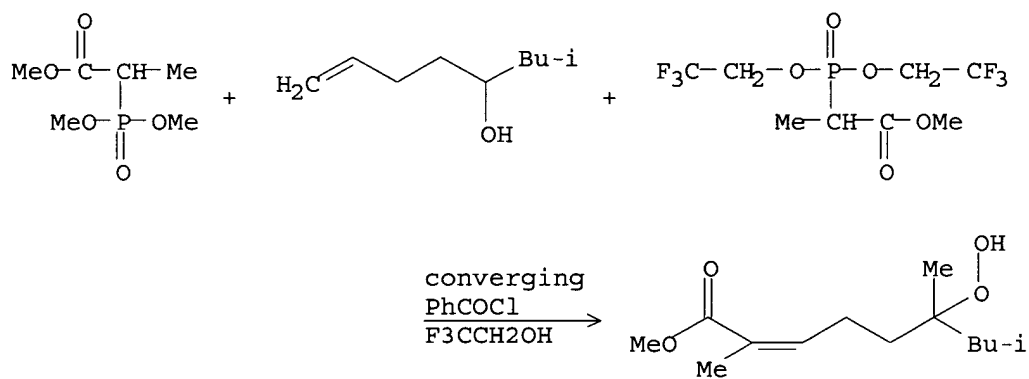
RX(623) OF 707 - 9 STEPS



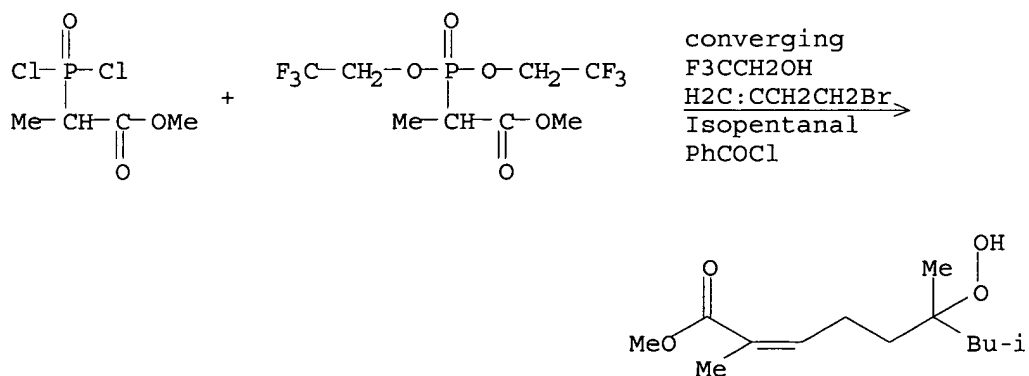
RX(627) OF 707 - 9 STEPS



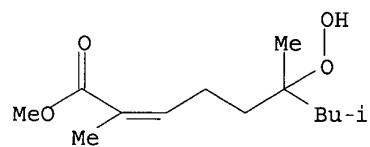
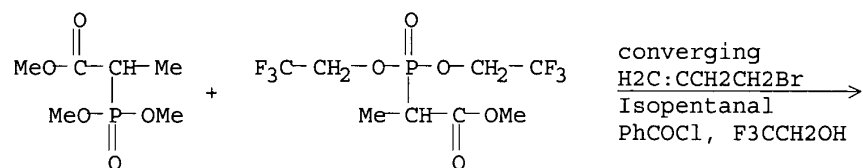
RX(629) OF 707 - 10 STEPS



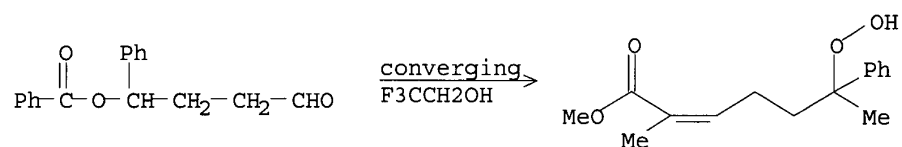
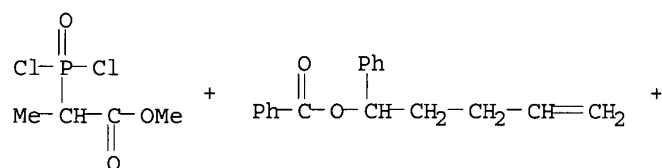
RX(633) OF 707 - 10 STEPS



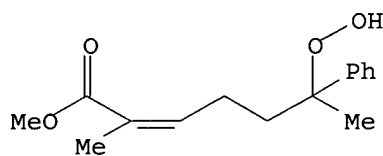
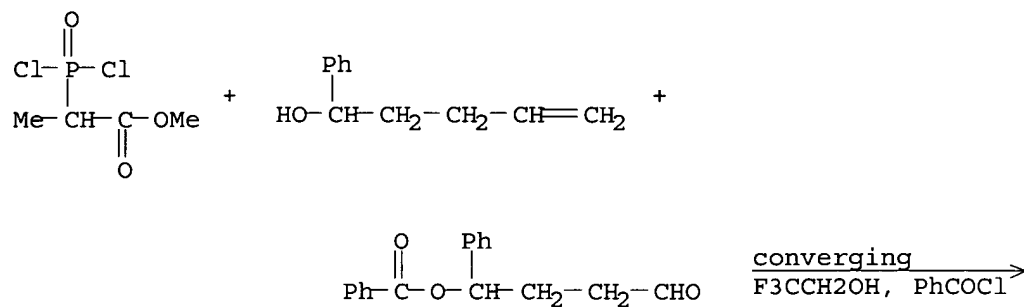
RX(635) OF 707 - 11 STEPS



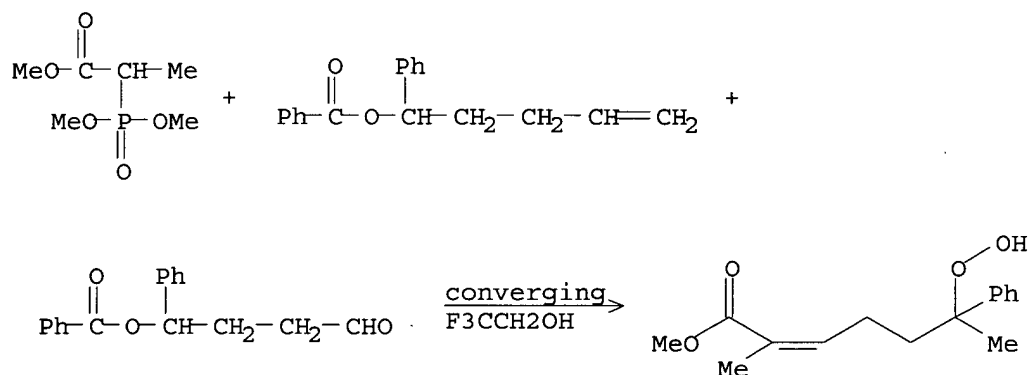
RX(658) OF 707 - 8 STEPS



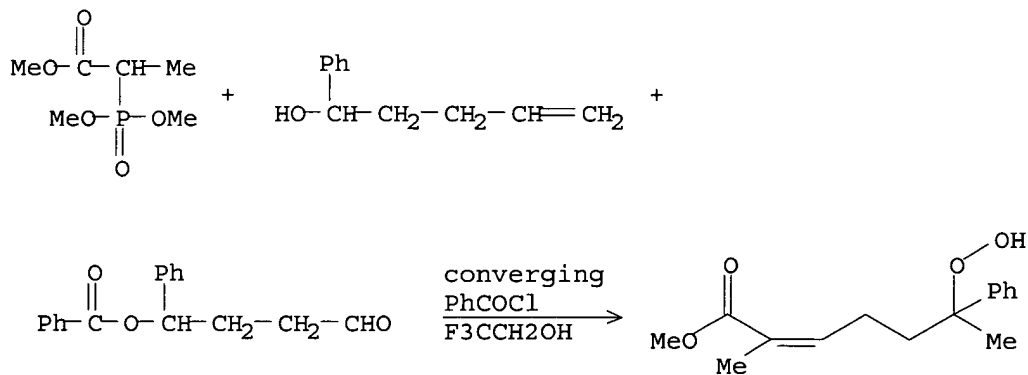
RX(660) OF 707 - 9 STEPS



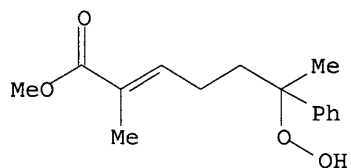
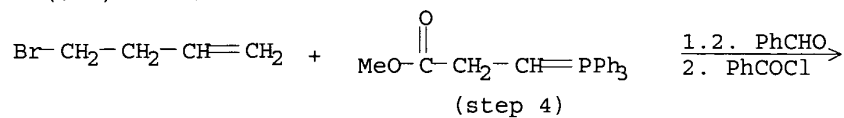
RX(670) OF 707 - 9 STEPS



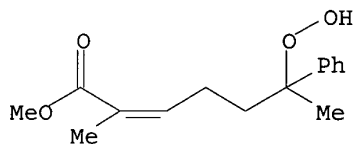
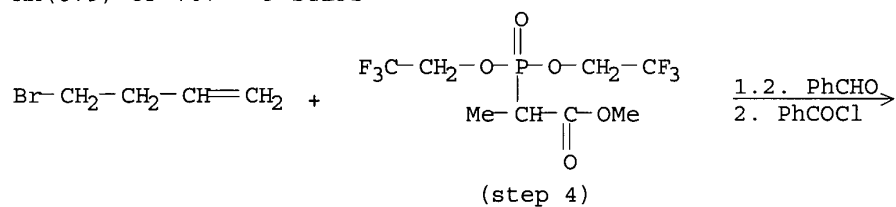
RX(672) OF 707 - 10 STEPS



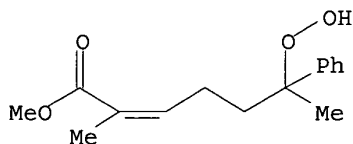
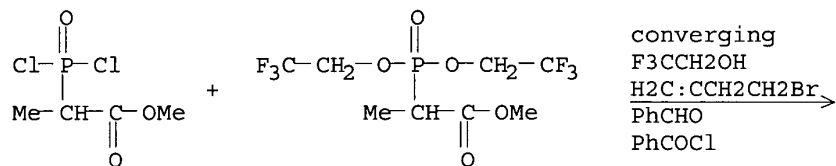
RX(677) OF 707 - 9 STEPS



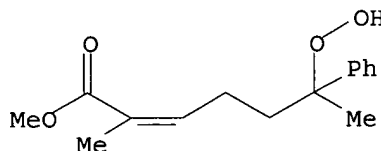
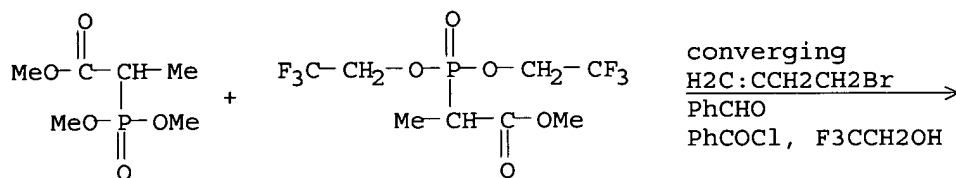
RX(679) OF 707 - 9 STEPS



RX(701) OF 707 - 10 STEPS



RX(703) OF 707 - 11 STEPS



L34 ANSWER 25 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

105:97096 CASREACT

TITLE:

Oxygenation of tert-butylphenols with an unsaturated side chain

AUTHOR(S):

Nishinaga, Akira; Iwasaki, Hitoshi; Shimizu, Tadashi; Toyoda, Yasushi; Matsuura, Teru

CORPORATE SOURCE:

Fac. Eng., Kyoto Univ., Kyoto, 606, Japan

SOURCE:

Journal of Organic Chemistry (1986), 51(12), 2257-66

CODEN: JOCEAH; ISSN: 0022-3263

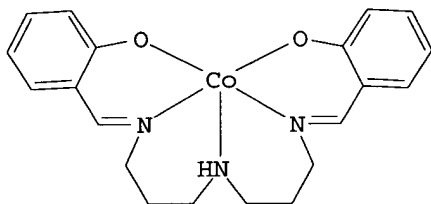
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

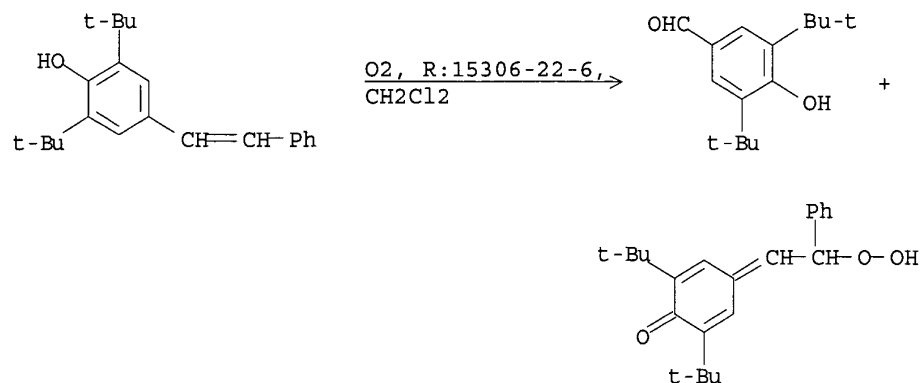


I

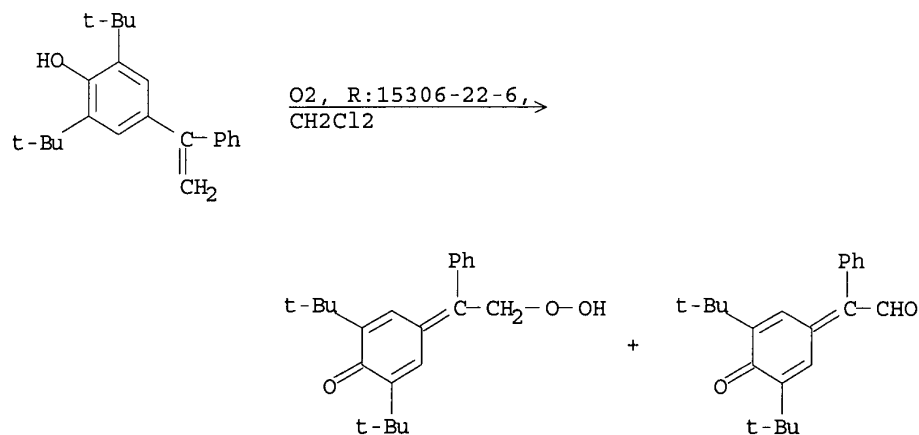
AB Base and Co(Salpr)(I)-promoted oxygenation of the title compds. was studied to obtain details concerning controlling factors in regioselective O<sub>2</sub> incorporation into phenols. In the oxygenation of 4-alkenyl-2,6-di-tert-butyl-(II) and 2-alkenyl-4,6-di-tert-butylphenols (III), the reactivity of the substrates and regioselectivity in the O<sub>2</sub> incorporation is interpreted in terms of electronic and steric effects of the alkenyl group as well as association effect of the countercation K<sup>+</sup> on the transition-state involving a charge-transfer from the substrate anion to O<sub>2</sub>. With 4-alkynyl-2,6-di-tert-butylphenols (IV), O<sub>2</sub> was incorporated exclusively into the ortho position only when the phenolate anion was associated with K<sup>+</sup>. On the contrary, in the oxygenation of II and III with

I, O<sub>2</sub> was incorporated exclusively into the alkenyl side chain, regardless of the nature of the substituent; with IV O<sub>2</sub> incorporation was distributed to both the ortho and the alkynyl side chain. The substituent-dependent regioselectivity in the oxygenation of phenols with I is because the reactive phenolate-Co(III) species undergo homolysis to form phenoxy radical-Co(II) species reversibly, whose oxygenations compete with each other. When the oxygenation of the anionic species predominates, O<sub>2</sub> is incorporated into the ortho position; with the radical species the para and side chain oxidns. predominate.

RX(30) OF 164

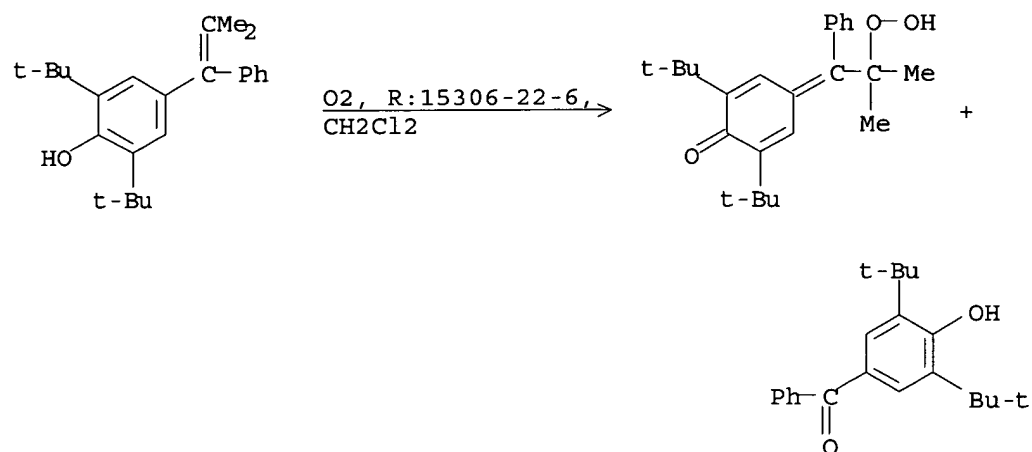


RX(31) OF 164

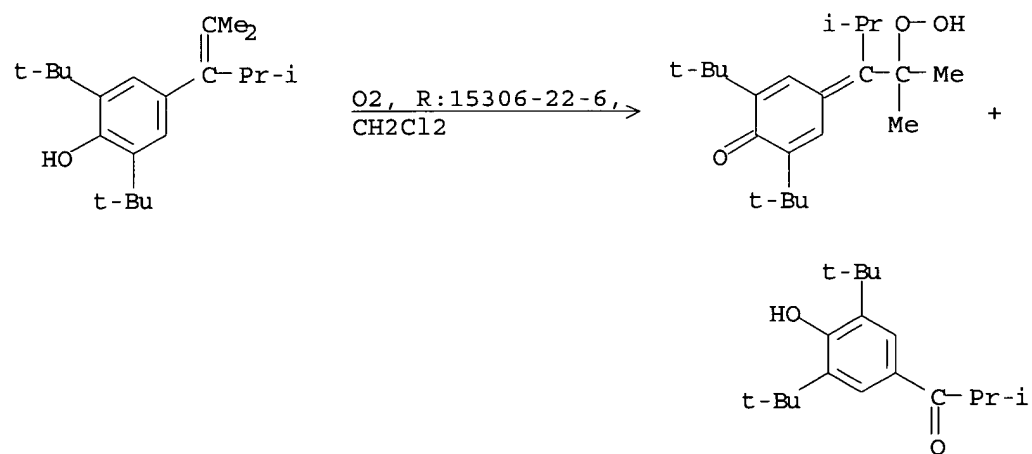




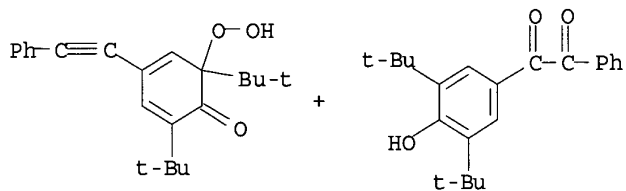
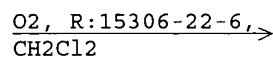
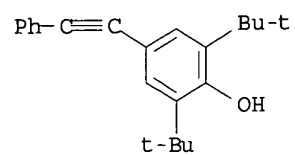
RX(32) OF 164



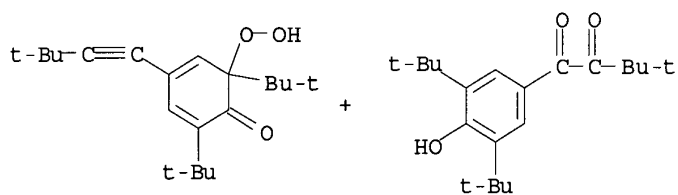
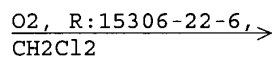
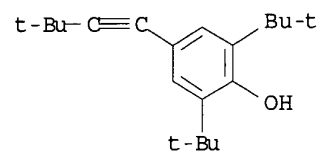
RX(33) OF 164



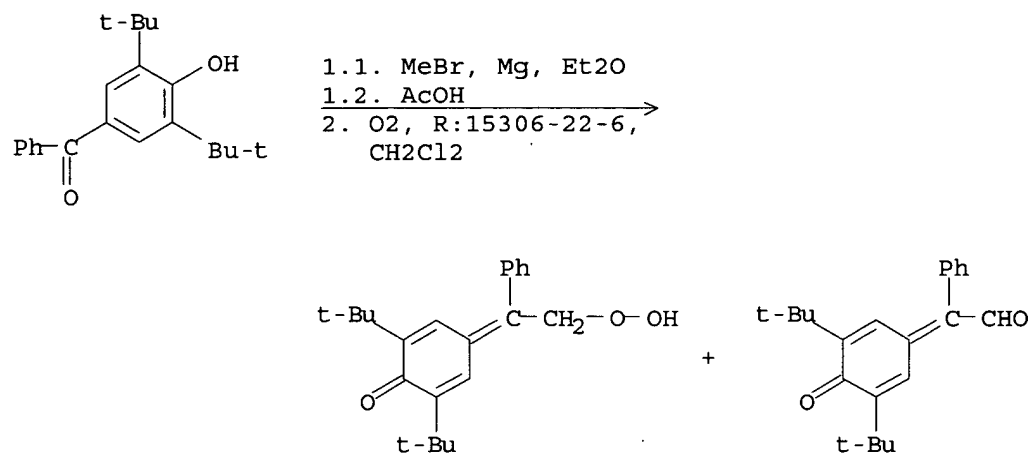
RX(64) OF 164



RX(66) OF 164

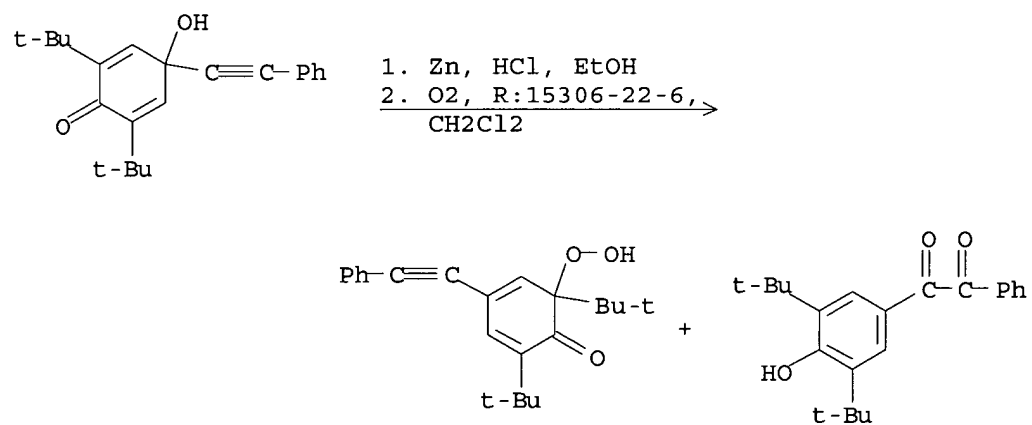


## RX(74) OF 164 - 2 STEPS

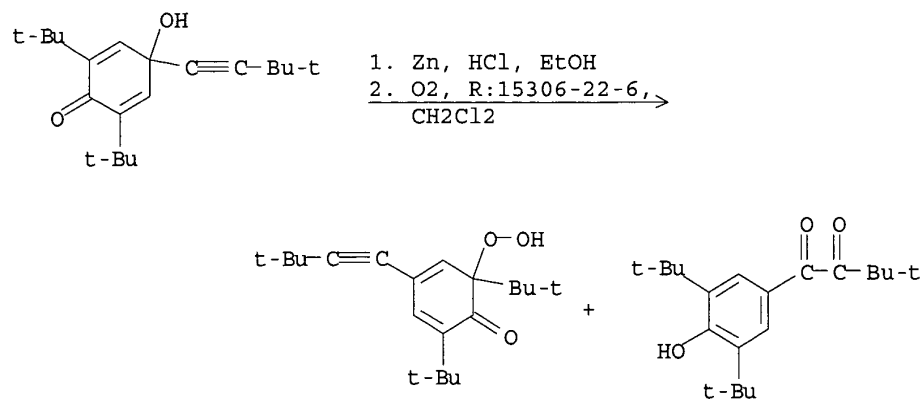


NOTE: 1) alkyl bromide assumed

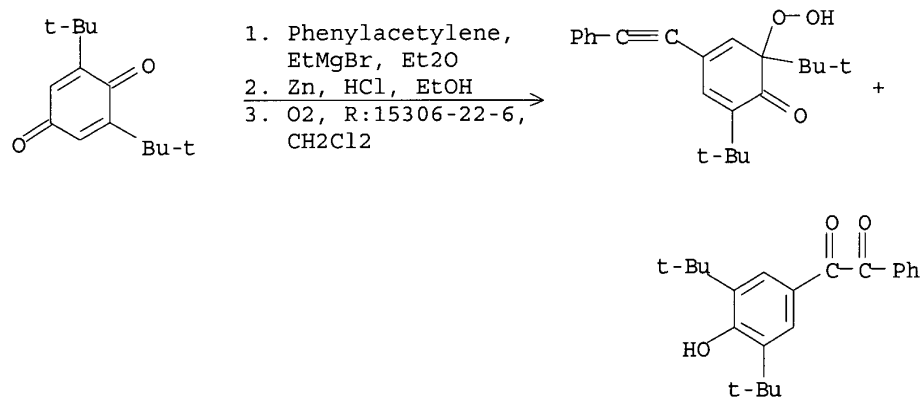
## RX(116) OF 164 - 2 STEPS



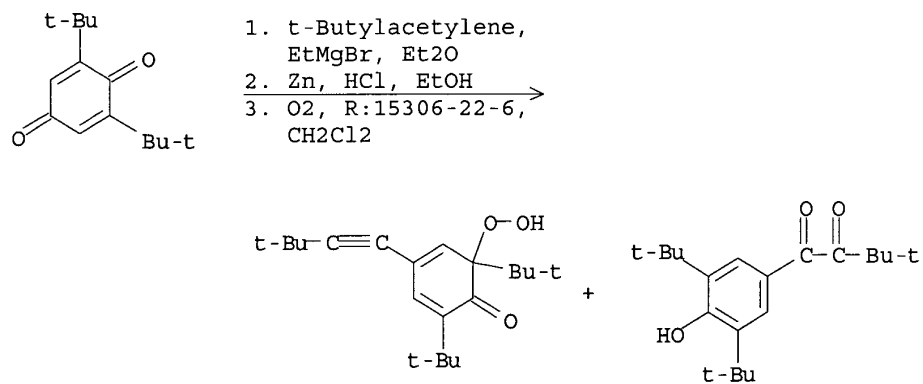
## RX(120) OF 164 - 2 STEPS



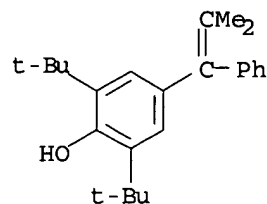
## RX(154) OF 164 - 3 STEPS



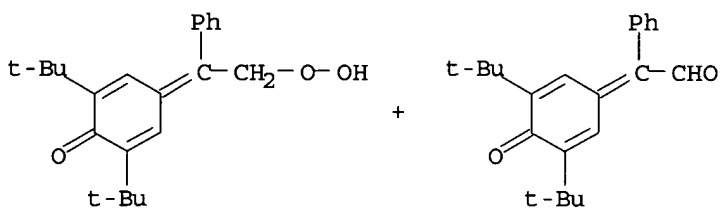
## RX(158) OF 164 - 3 STEPS



## RX(161) OF 164 - 3 STEPS

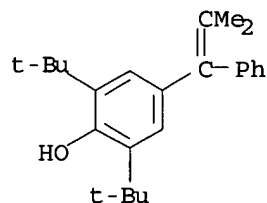


1. O<sub>2</sub>, R:15306-22-6,  
CH<sub>2</sub>Cl<sub>2</sub>
- 2.1. MeBr, Mg, Et<sub>2</sub>O
- 2.2. AcOH
3. O<sub>2</sub>, R:15306-22-6,  
CH<sub>2</sub>Cl<sub>2</sub>

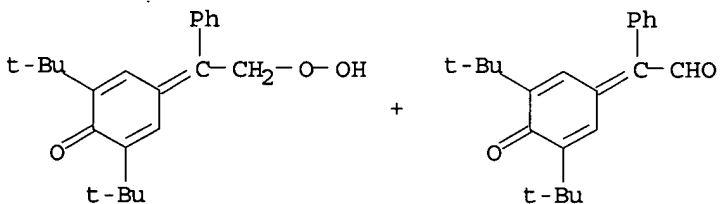


NOTE: 2) alkyl bromide assumed

## RX(162) OF 164 - 3 STEPS



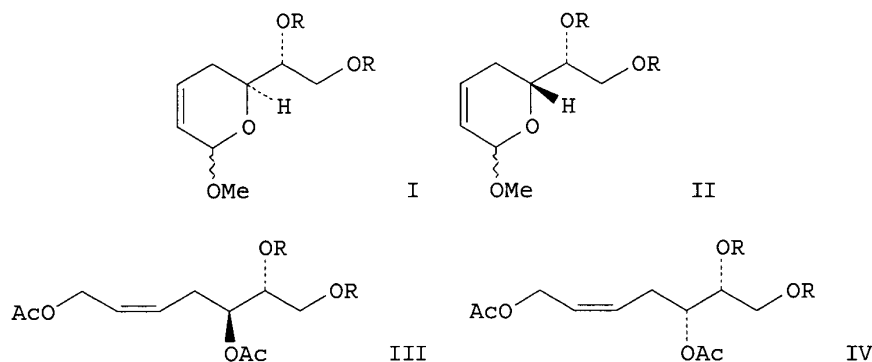
1. O<sub>2</sub>, t-BuOK, DMF
- 2.1. MeBr, Mg, Et<sub>2</sub>O
- 2.2. AcOH
3. O<sub>2</sub>, R:15306-22-6,  
CH<sub>2</sub>Cl<sub>2</sub>



NOTE: 2) alkyl bromide assumed

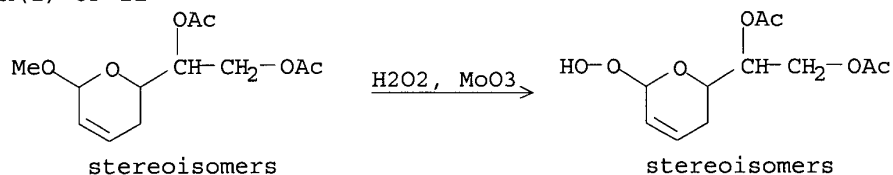
L34 ANSWER 26 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 106:102630 CASREACT  
 TITLE: Novel reductive opening of 5,6-dihydro-2H-pyran ring  
 AUTHOR(S): Jurczak, Janusz; Bauer, Tomasz; Ankner, Kjell  
 CORPORATE SOURCE: Inst. Org. Chem., Pol. Acad. Sin., Warsaw, 01-224,  
 Pol.  
 SOURCE: Heterocycles (1986), 24(6), 1531-4  
 CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

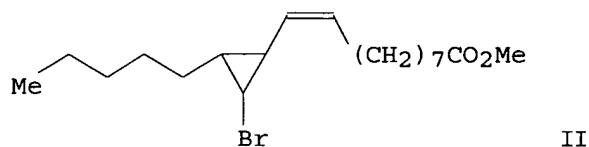
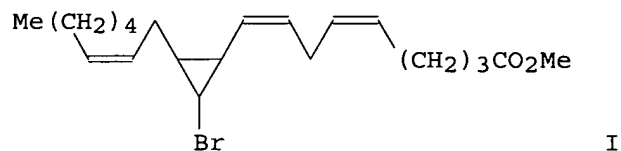


AB Methoxydihydropyrans I (R = Ac, PhCH<sub>2</sub>) and II (R = Ac, PhCH<sub>2</sub>) on oxidation with H<sub>2</sub>O<sub>2</sub> in the presence of MoO<sub>3</sub>, followed by reduction of the resulting peroxides with NaBH<sub>4</sub> and then acetylation with Ac<sub>2</sub>O gave enantiomerically pure open-chain compds. III and IV (same R), resp. III and IV can serve as chiral building blocks in the synthesis of natural products.

RX(1) OF 11

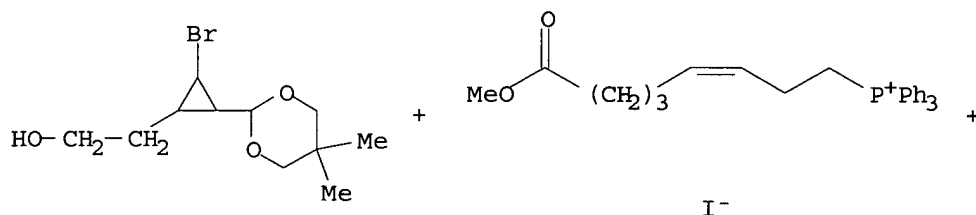


L34 ANSWER 27 OF 76 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 103:122958 CASREACT  
 TITLE: General synthesis of polyunsaturated fatty acid hydroperoxides involving a novel vinylcyclopropyl bromide ring opening  
 AUTHOR(S): Porter, N. A.; Ziegler, C. B., Jr.; Khouri, F. F.; Roberts, D. H.  
 CORPORATE SOURCE: P. M. Gross Chem. Lab., Duke Univ., Durham, NC, 27706, USA  
 SOURCE: Journal of Organic Chemistry (1985), 50(13), 2252-8  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



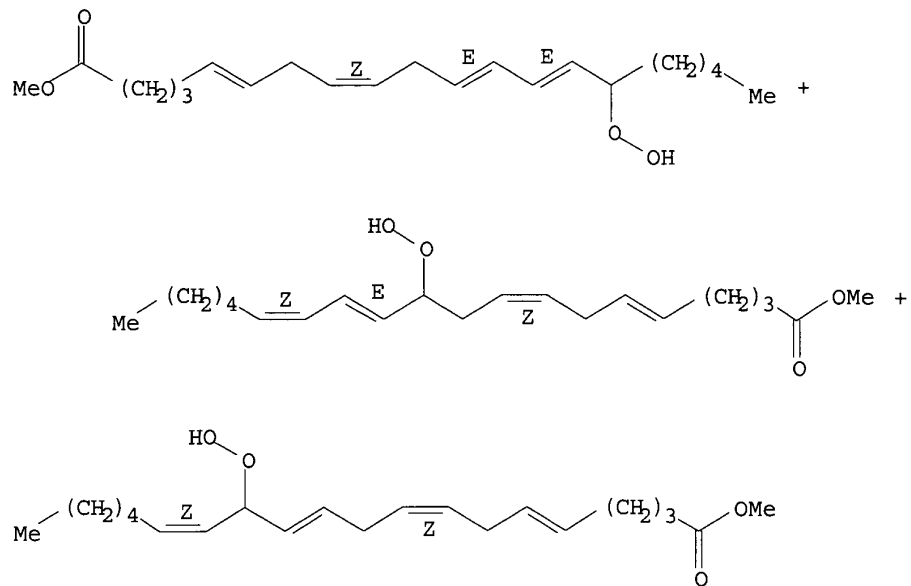
AB A variety of 18- and 20-carbon polyunsatd. fatty acid hydroperoxides were synthesized via an orbital symmetry controlled ring opening of vinylcyclopropyl bromides. Six 20-carbon vinylcyclopropyl bromides, e.g. I were synthesized by a route starting from 2-ethoxy-Δ<sup>3,5</sup>-dihydropyran and an 18-carbon vinylcyclopropyl bromide II by a route starting from propargyl alc. All six vinylcyclopropyl bromides underwent facile Ag<sup>+</sup>-assisted ring opening in the presence of excess H<sub>2</sub>O<sub>2</sub> to form the target fatty acid hydroperoxide isomers in good yields. In most cases the products were produced with stereochem. control. The product hydroperoxides formed in this ring-opening reaction are consistent with a mechanism involving the formation of a pentadienyl cation intermediate. A minor product found in the reaction of II provides evidence that homoallylic participation by alkenyl substituents can change the course of the electrocyclic ring opening.

RX(102) OF 133 - 5 STEPS

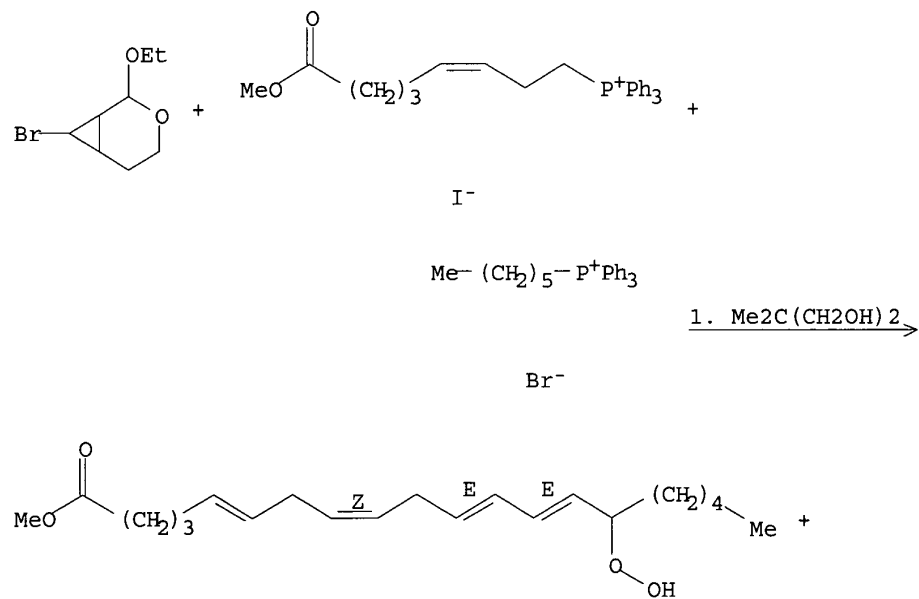


- Me<sup>-</sup> (CH<sub>2</sub>)<sub>5</sub> - P<sup>+</sup>Ph<sub>3</sub>
- Br<sup>-</sup>
1. AcONa, PCC, CH<sub>2</sub>Cl<sub>2</sub>, N<sub>2</sub>
  - 2.1. t-BuOK, N<sub>2</sub>, THF
  - 2.2. THF
  3. HCO<sub>2</sub>H, THF, N<sub>2</sub>
  - 4.1. t-BuOK, THF, N<sub>2</sub>
  5. H<sub>2</sub>O<sub>2</sub>, F<sub>3</sub>CCO<sub>2</sub> Ag, Et<sub>2</sub>O

RX(102) OF 133 - 5 STEPS

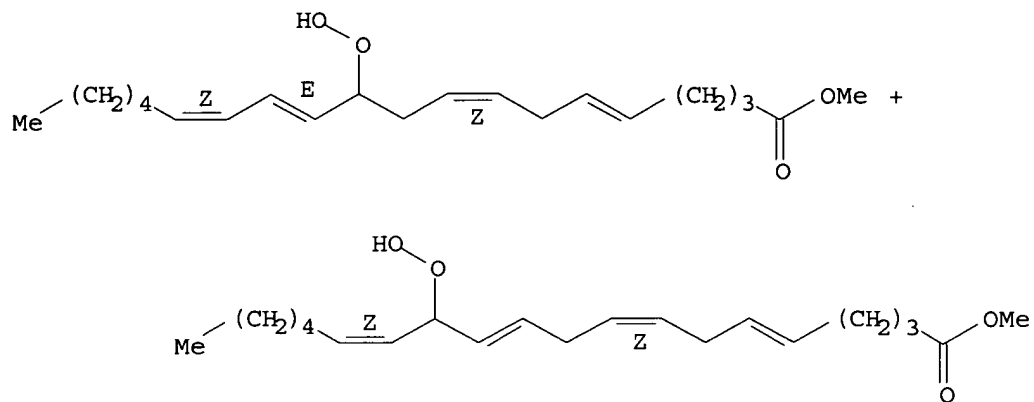


RX(103) OF 133 - 6 STEPS

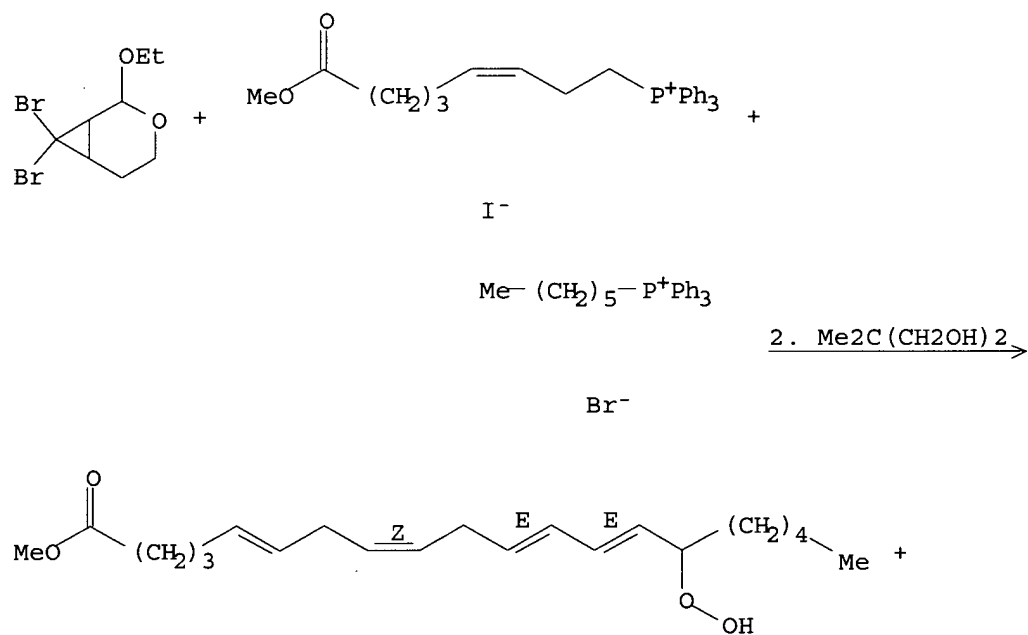




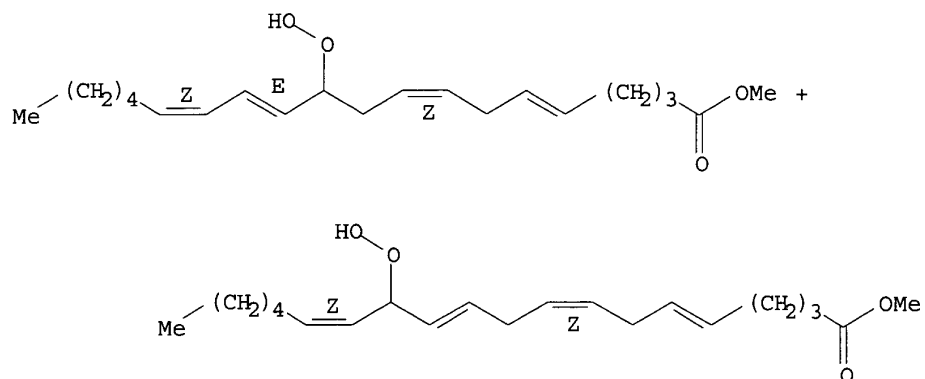
RX(103) OF 133 - 6 STEPS



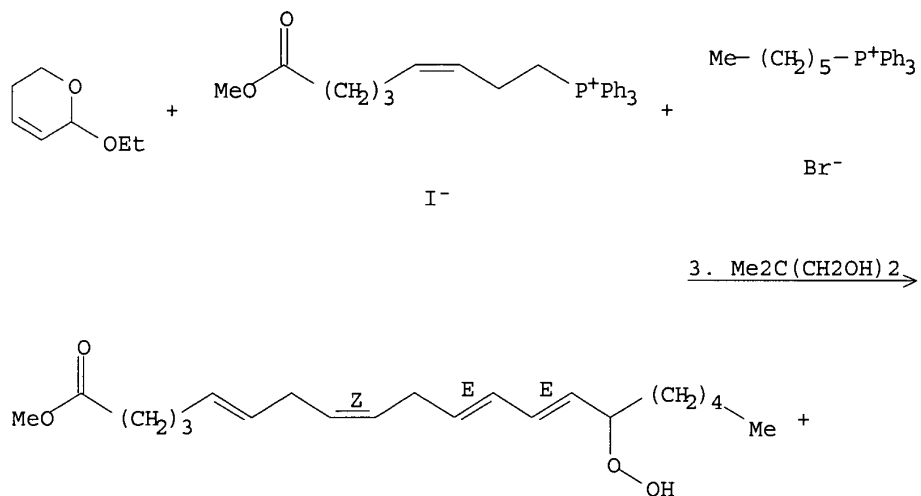
RX(104) OF 133 - 7 STEPS



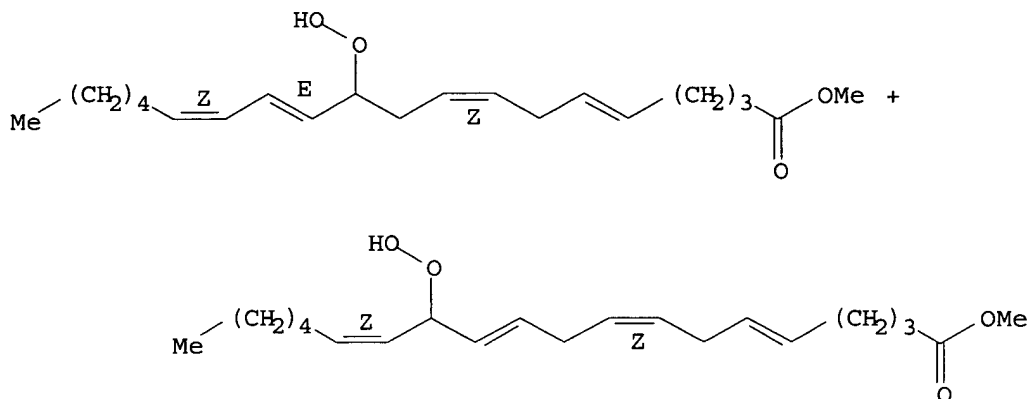
RX(104) OF 133 - 7 STEPS



RX(105) OF 133 - 8 STEPS



RX(105) OF 133 - 8 STEPS



L34 ANSWER 28 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 102:203393 CASREACT

TITLE: Enhanced endo-exo selectivity in the stereochemistry of ketonization of enols. Part 201

AUTHOR(S): Zimmerman, Howard E.; Linder, Linus W.

CORPORATE SOURCE: Dep. Chem., Univ. Wisconsin, Madison, WI, 53706, USA

SOURCE: Journal of Organic Chemistry (1985), 50(10), 1637-46

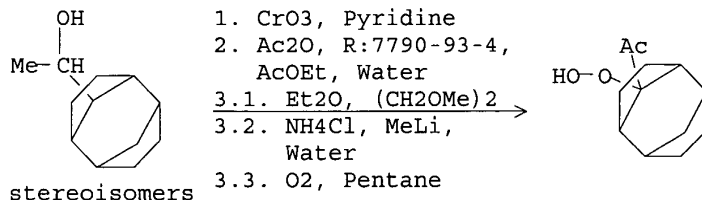
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

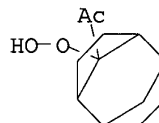
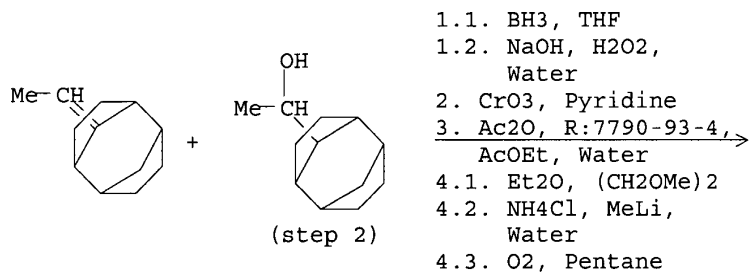
AB The enols of 9-acetyl-anti-tricyclo[4.2.1.1<sup>2,5</sup>]decane (I) and 9-benzoyl-anti-tricyclo[4.2.1.1<sup>2,5</sup>]decane (II) were generated by reaction of the bromo ketone with mercaptans or with dilute HI in acetone, or by conversion of the enol acetates to the enolates followed by protonation. The enol of I was also generated by photolysis of the enolxy dimer (III). The enols were stable with half-lives ranging from a half hour to more than 24 h, depending on conditions. The presence of the enols was monitored by reaction with O<sub>2</sub>. III was formed when the α-bromo(acetyl)tricyclic was irradiated in Me<sub>2</sub>CHOH containing NaOAc; III had two enolxy radicals bonded from the C(α) atom of one to the enolxy oxygen of the second. Base-catalyzed equilibration of the ketones led to the endo and the exo isomers with a product ratio less than 1 to 1000. Enol ketonization occurs with exo attack, giving the endo isomers, (the endo isomers are preferred by at least 3300 to 1). The very large kinetic preference for the less stable endo ketone isomer results from steric hindrance by the C(3) and C(5) axial CH<sub>2</sub> groups blocking the endo approach of proton donors. A MM2 treatment of the stereochem. of ketonization revealed the expected preference for exo protonation of both the tricyclic enol (observed in the present study) and also unsubstituted exocyclic 6-ring enols. For the 2-phenyl-1-acetyl system, the axial Ph conformer of starting material was preferred. However, for the protonation transition state, the equatorial Ph conformer with exo protonation was lowest in energy. Next was the axial Ph conformer with axial protonation. Third was the axial Ph conformer with exo protonation, and least stable was the equatorial Ph conformer with endo protonation.

## RX(103) OF 447 - 3 STEPS

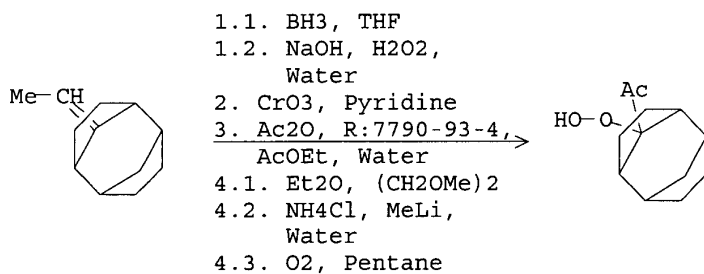


stereoisomers

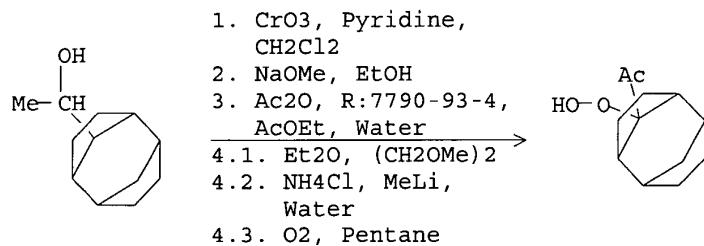
## RX(104) OF 447 - 4 STEPS



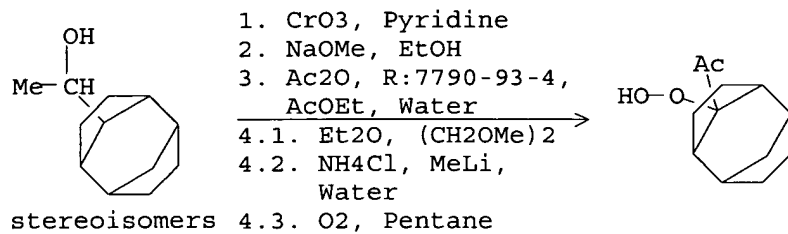
## RX(105) OF 447 - 4 STEPS



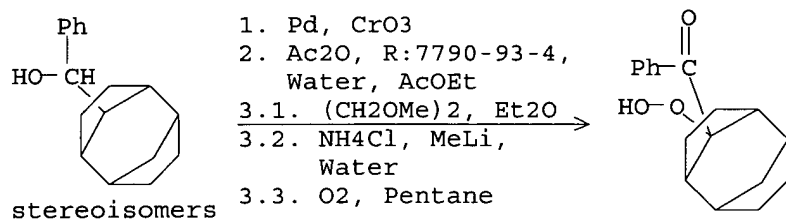
## RX(106) OF 447 - 4 STEPS



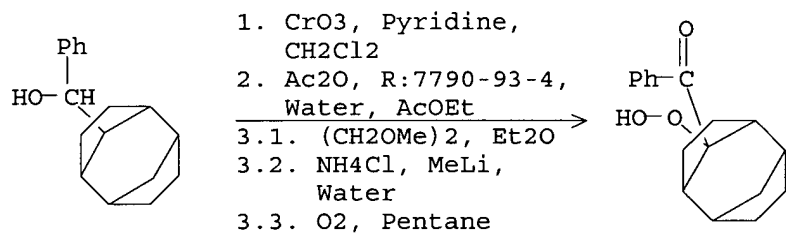
## RX(112) OF 447 - 4 STEPS



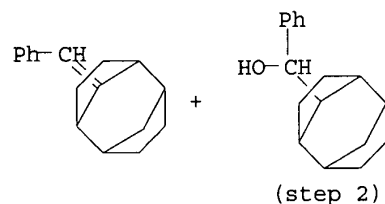
## RX(169) OF 447 - 3 STEPS



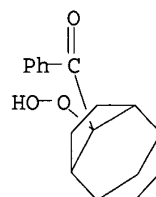
## RX(170) OF 447 - 3 STEPS



RX(173) OF 447 - 4 STEPS

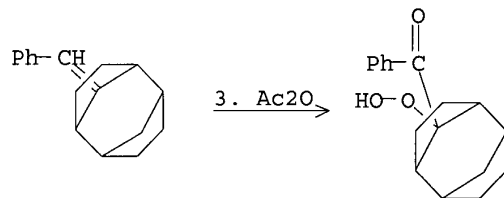


- 1.1. BH<sub>3</sub>, THF
- 1.2. NaOH, H<sub>2</sub>O<sub>2</sub>,  
Water
2. Pd, CrO<sub>3</sub>
3. Ac<sub>2</sub>O, R:7790-93-4,  
Water, AcOEt
- 4.1. (CH<sub>2</sub>OMe)<sub>2</sub>, Et<sub>2</sub>O
- 4.2. NH<sub>4</sub>Cl, MeLi,  
Water
- 4.3. O<sub>2</sub>, Pentane



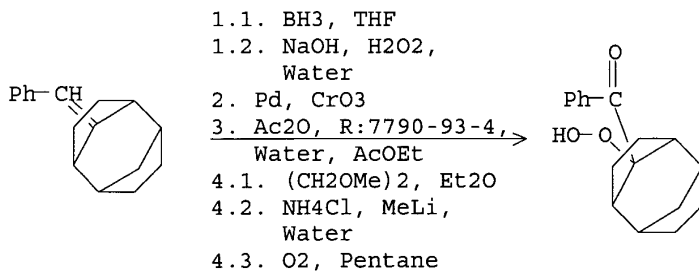
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(174) OF 447 - 4 STEPS



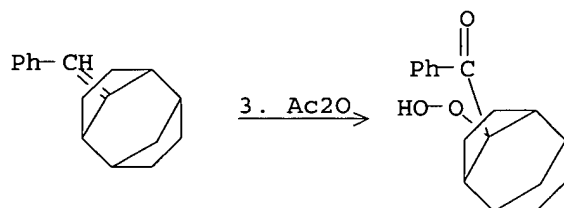
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(175) OF 447 - 4 STEPS



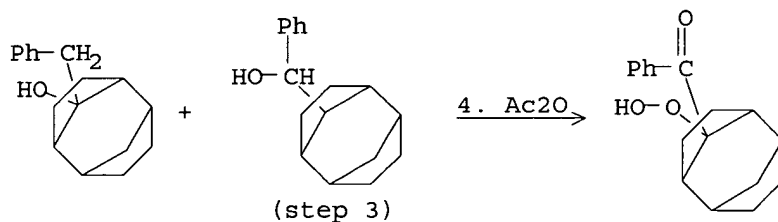
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(176) OF 447 - 4 STEPS



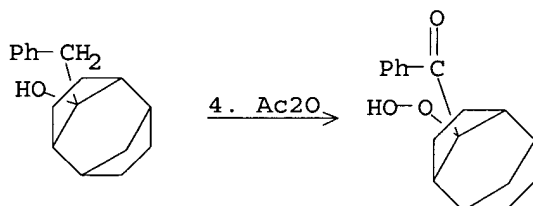
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(313) OF 447 - 5 STEPS



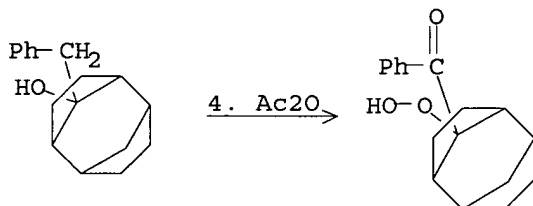
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(314) OF 447 - 5 STEPS



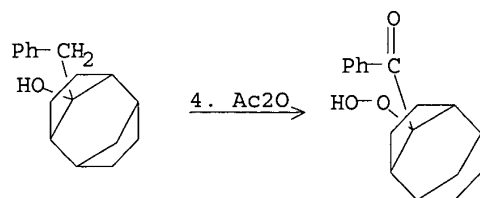
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(315) OF 447 - 5 STEPS



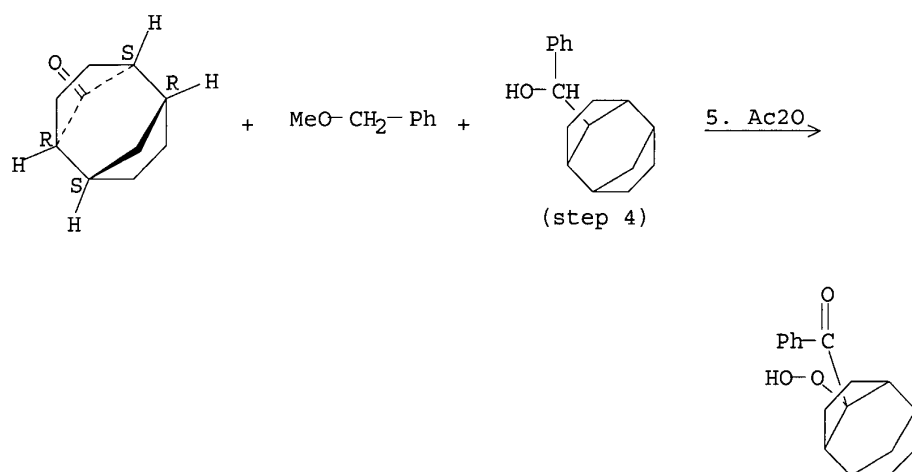
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(316) OF 447 - 5 STEPS



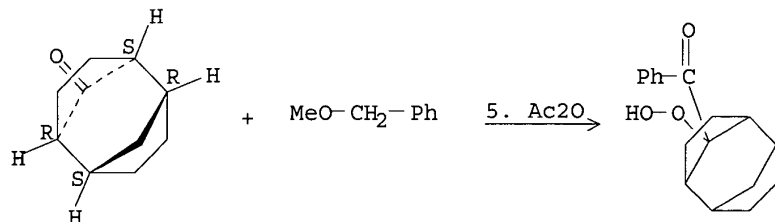
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(329) OF 447 - 6 STEPS



NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

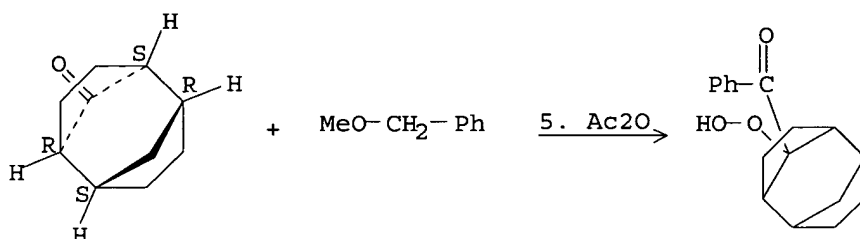
RX(330) OF 447 - 6 STEPS



NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

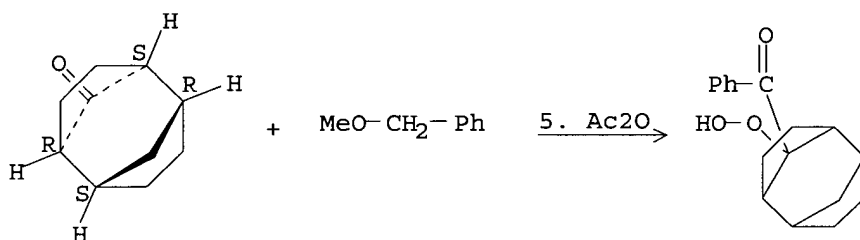


RX(331) OF 447 - 6 STEPS



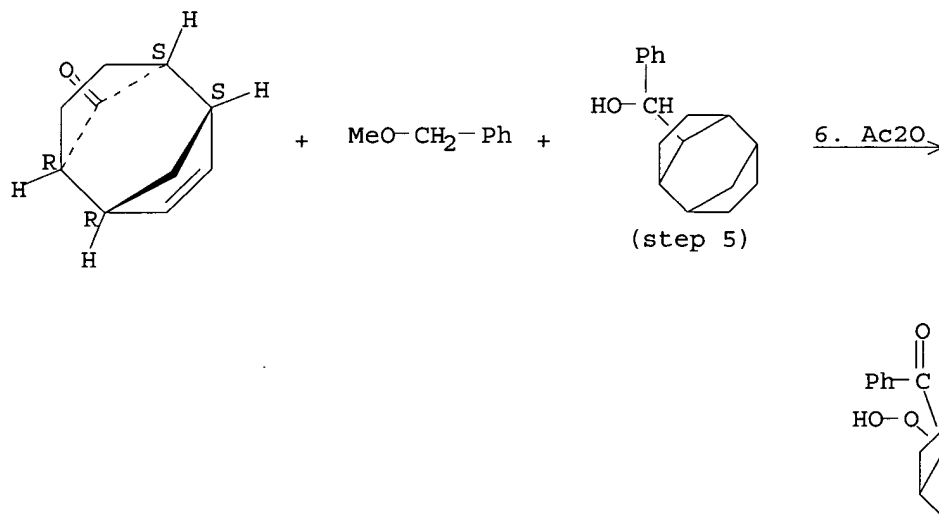
NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

RX(332) OF 447 - 6 STEPS



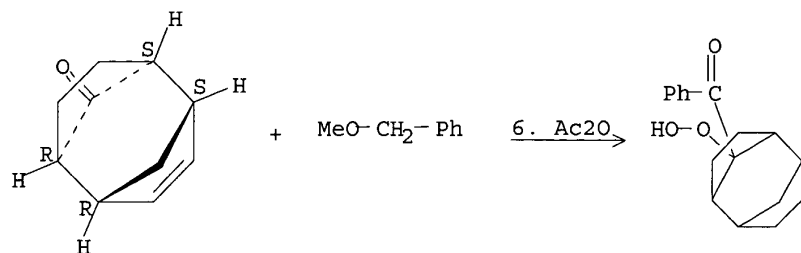
NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

RX(345) OF 447 - 7 STEPS



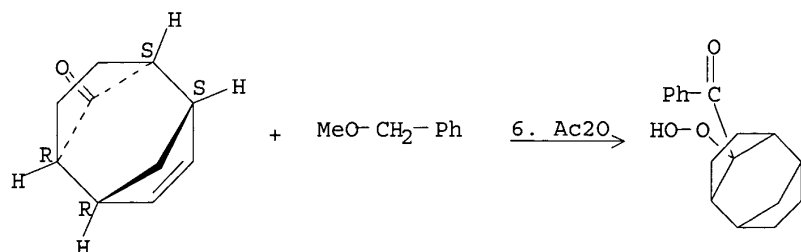
NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(346) OF 447 - 7 STEPS



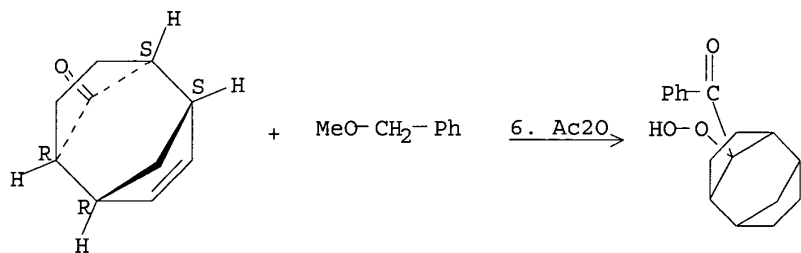
NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(347) OF 447 - 7 STEPS



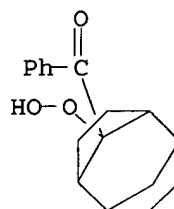
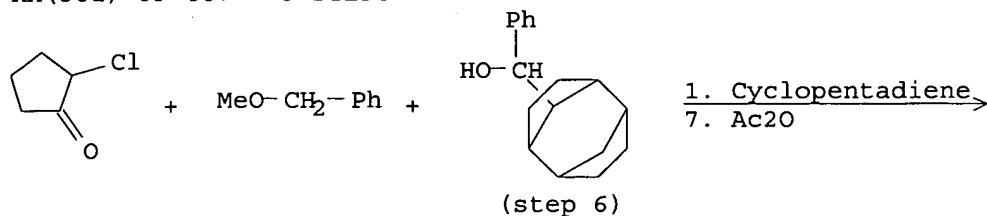
NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(348) OF 447 - 7 STEPS



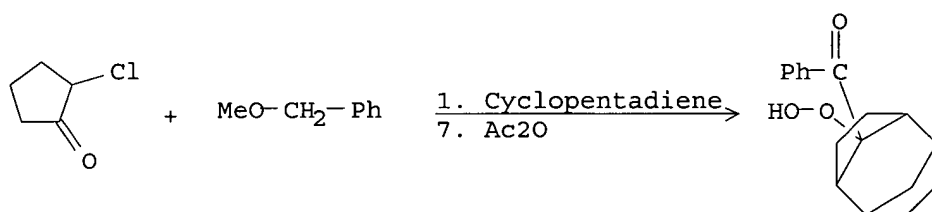
NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(361) OF 447 - 8 STEPS



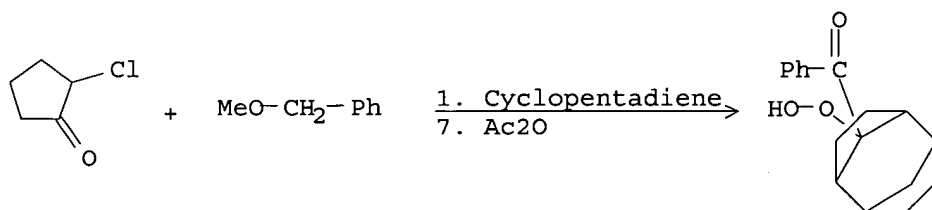
NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

RX(362) OF 447 - 8 STEPS



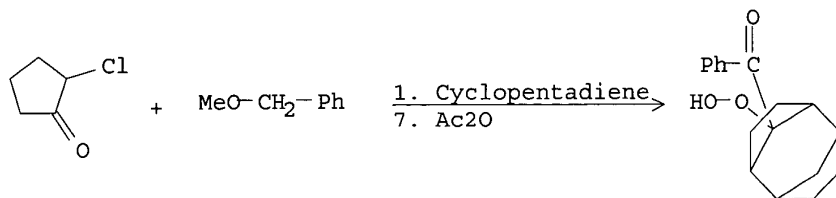
NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

RX(363) OF 447 - 8 STEPS



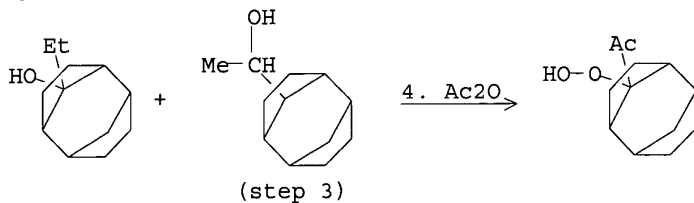
NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

RX(364) OF 447 - 8 STEPS

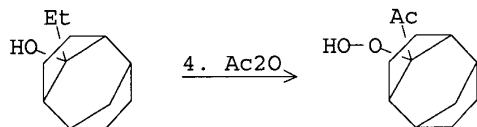


NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

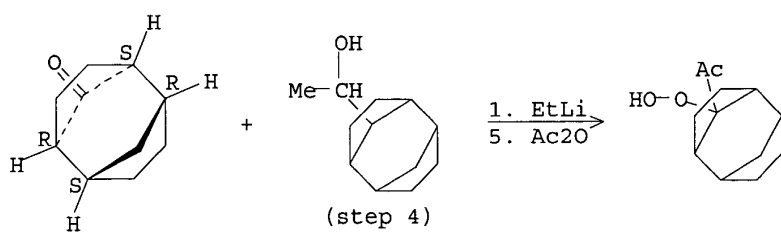
RX(381) OF 447 - 5 STEPS



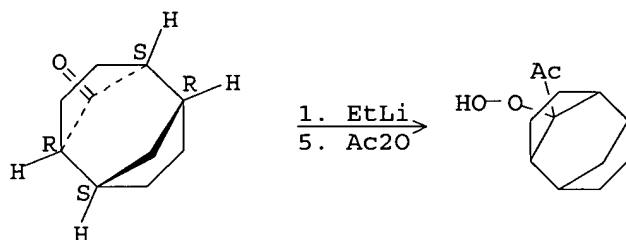
RX(382) OF 447 - 5 STEPS



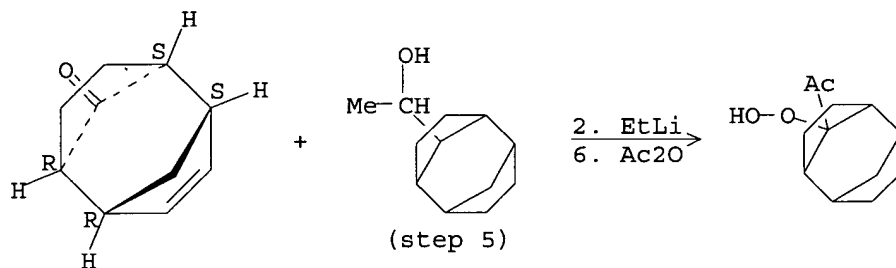
RX(387) OF 447 - 6 STEPS



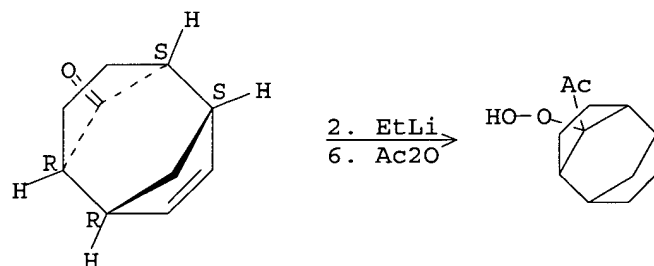
RX(388) OF 447 - 6 STEPS



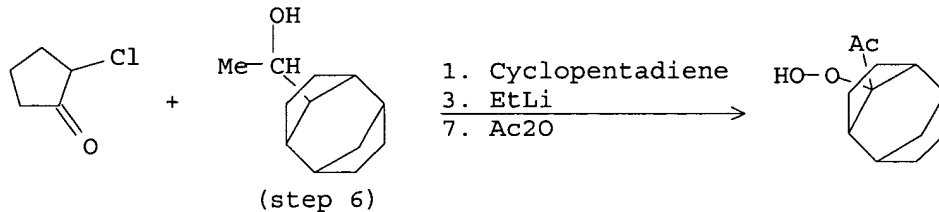
RX(393) OF 447 - 7 STEPS



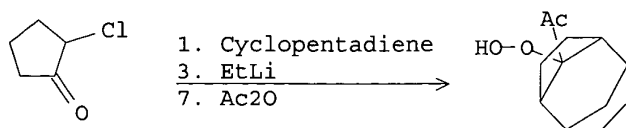
RX(394) OF 447 - 7 STEPS



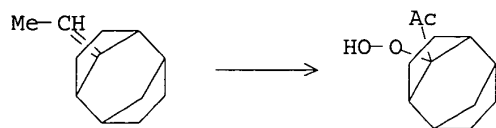
RX(399) OF 447 - 8 STEPS



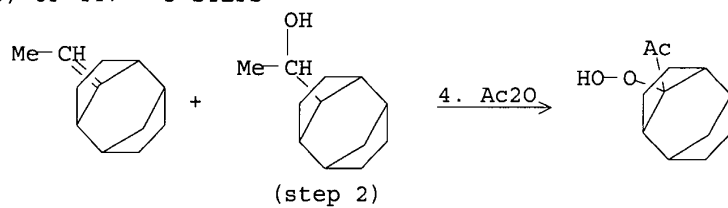
RX(400) OF 447 - 8 STEPS



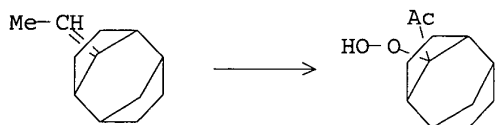
RX(405) OF 447 - 5 STEPS



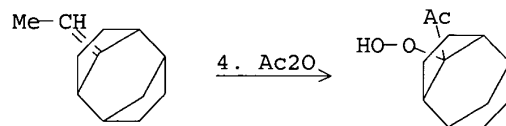
RX(406) OF 447 - 5 STEPS



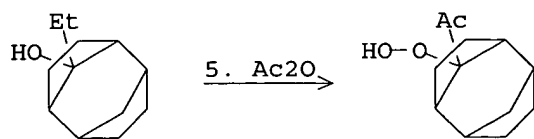
RX(407) OF 447 - 5 STEPS



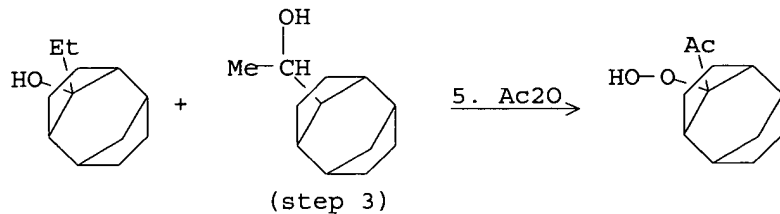
RX(408) OF 447 - 5 STEPS



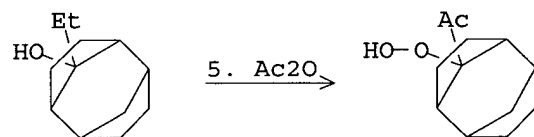
RX(409) OF 447 - 6 STEPS



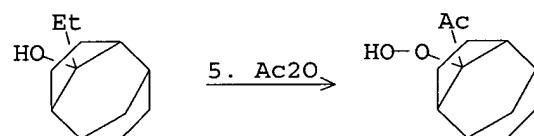
RX(410) OF 447 - 6 STEPS



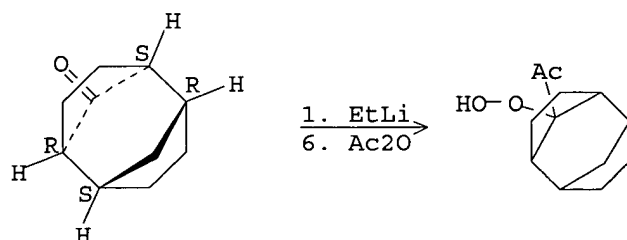
RX(411) OF 447 - 6 STEPS



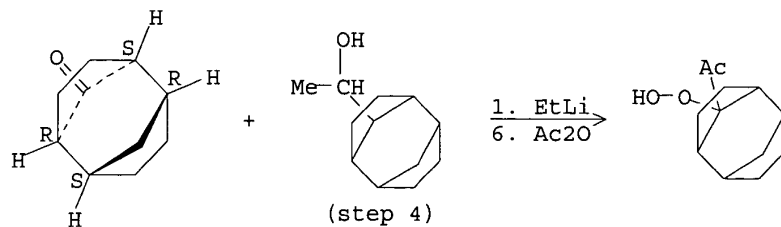
RX(412) OF 447 - 6 STEPS



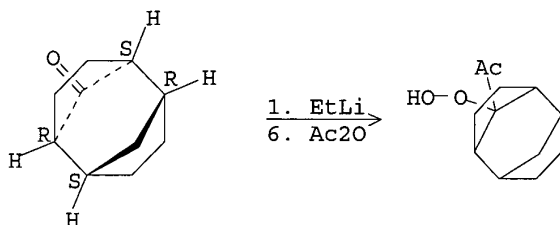
RX(413) OF 447 - 7 STEPS



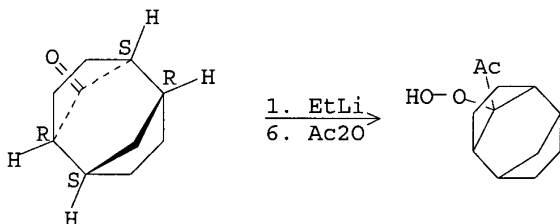
RX(414) OF 447 - 7 STEPS



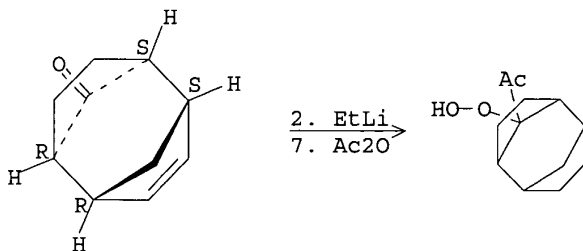
RX(415) OF 447 - 7 STEPS



RX(416) OF 447 - 7 STEPS

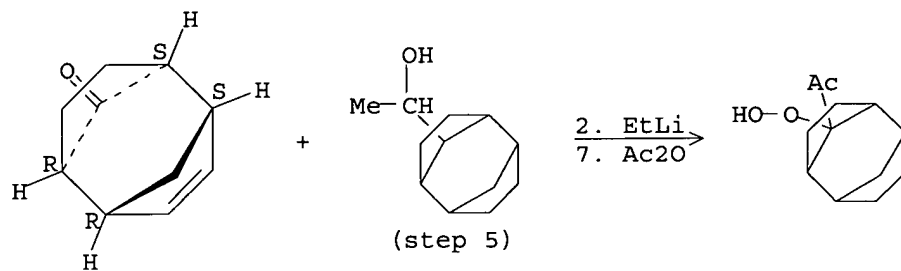


RX(417) OF 447 - 8 STEPS

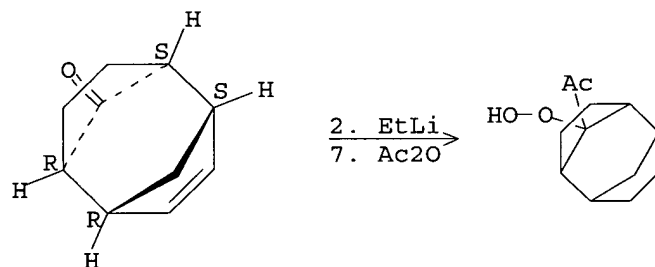




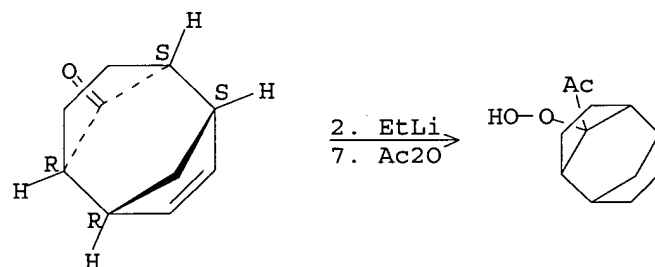
RX(418) OF 447 - 8 STEPS



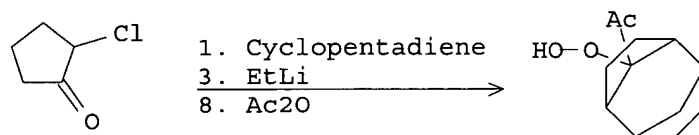
RX(420) OF 447 - 8 STEPS



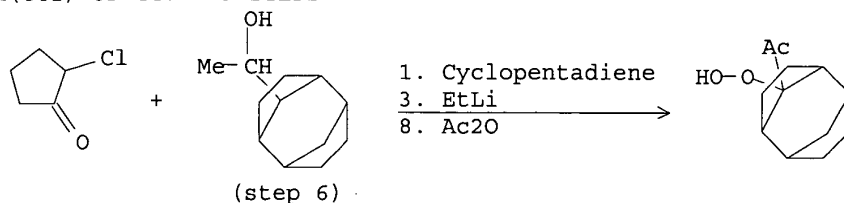
RX(421) OF 447 - 8 STEPS



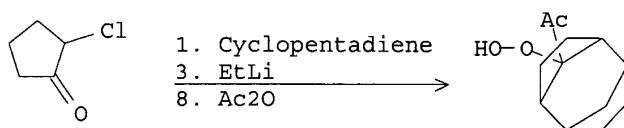
RX(440) OF 447 - 9 STEPS



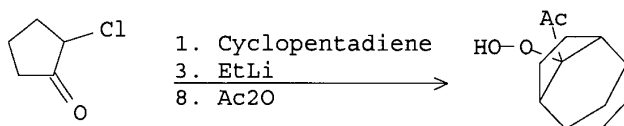
RX(441) OF 447 - 9 STEPS



RX(442) OF 447 - 9 STEPS



RX(443) OF 447 - 9 STEPS



L34 ANSWER 29 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

99:21926 CASREACT

TITLE:

The synthesis of 11R- and 11S-HETE [(5Z, 8Z, 12E, 14Z)-11-hydroxyeicosatetraenoic acid] and of 11-R,S-HPETE [(5Z, 8Z, 12E, 14Z)-11-hydroperoxyeicosatetraenoic acid] methyl esters

AUTHOR(S):

Just, George; Luthe, Corinne; Viet, Minh Tan Phan

CORPORATE SOURCE:

Dep. Chem., McGill Univ., Montreal, QC, H3A 2K6, Can.

SOURCE:

Canadian Journal of Chemistry (1983), 61(4), 712-17  
CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE:

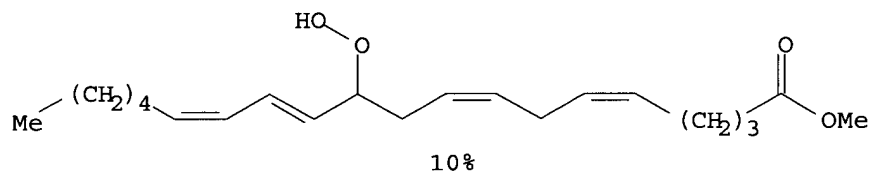
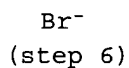
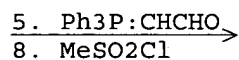
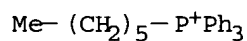
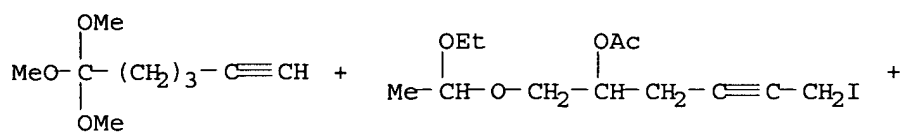
Journal

LANGUAGE:

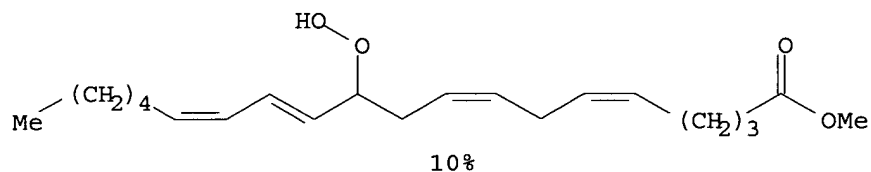
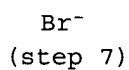
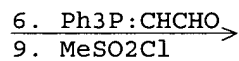
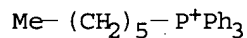
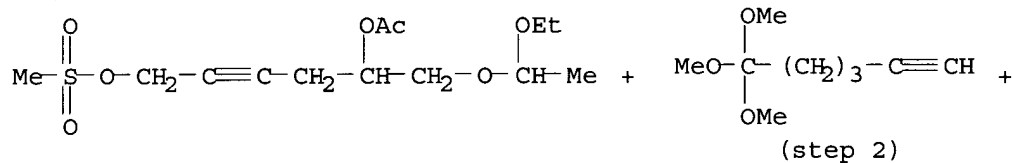
English

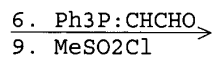
AB Me (11R)- and (11S)-hydroxyeicosa-(5Z,8Z,12E,14Z)-tetraenoate (S-I) and the corresponding 11-hydroperoxide were prepared from readily available starting materials. <sup>1</sup>H nmr studies of I were undertaken to confirm the structure. Some conformational properties are discussed.

RX(202) OF 223 - 9 STEPS

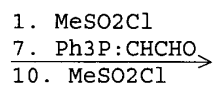


RX(204) OF 223 - 10 STEPS

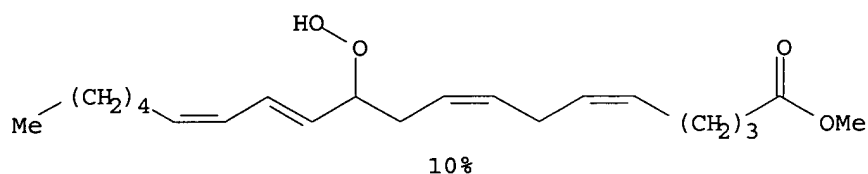
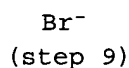
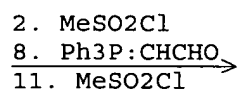
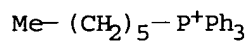
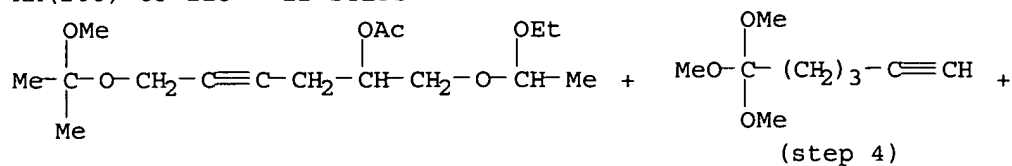


$$\begin{array}{c} \text{OMe} \\ | \\ \text{MeO}-\text{C}-(\text{CH}_2)_3-\text{C}\equiv\text{CH} \\ | \\ \text{OMe} \end{array} + \begin{array}{c} \text{OEt} \quad \quad \text{OAc} \\ | \quad \quad | \\ \text{Me}-\text{CH}-\text{O}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{C}\equiv\text{C}-\text{CH}_2\text{I} \end{array} +$$
CCCCC/C=C/C(=O)O/C=C/C=C/C(=O)OCC
$$\begin{array}{c} \text{OEt} \qquad \text{OAc} \\ | \qquad \quad | \\ \text{Me}-\text{CH}-\text{O}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{C}\equiv\text{C}-\text{CH}_2-\text{OH} \end{array} + \begin{array}{c} \text{OMe} \\ | \\ \text{MeO}-\text{C}-(\text{CH}_2)_3-\text{C}\equiv\text{CH} \\ | \\ \text{OMe} \end{array} +$$

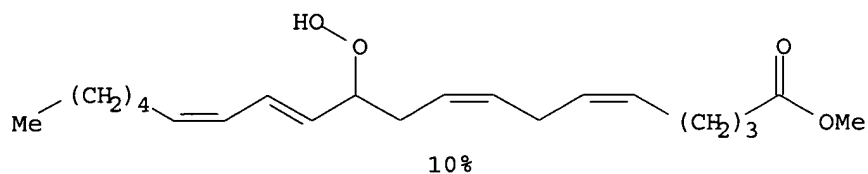
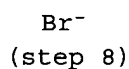
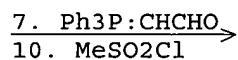
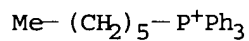
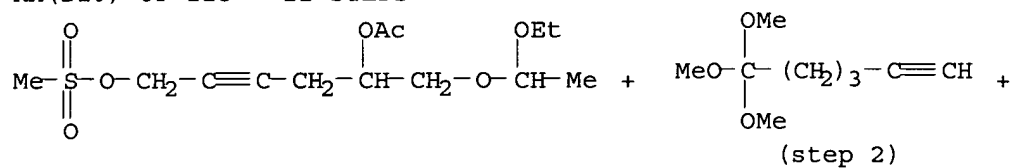
(step 3)

CCCCC/C=C/C(=O)OCC/C=C/C/C=C/C(=O)OCC

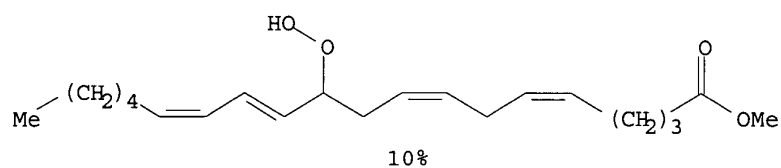
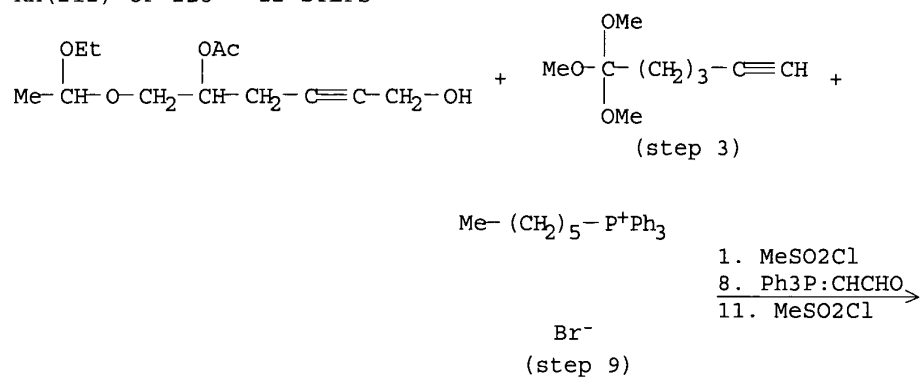
RX(208) OF 223 - 12 STEPS



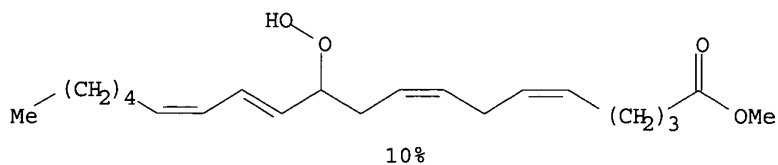
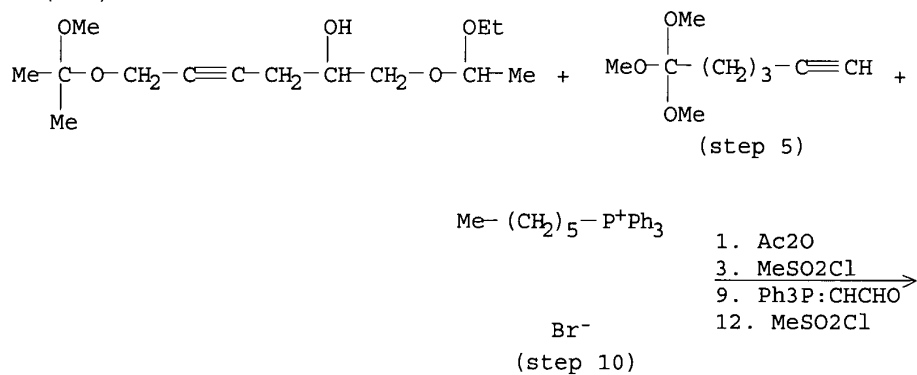
RX(210) OF 223 - 11 STEPS



RX(212) OF 223 - 12 STEPS

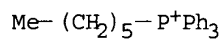
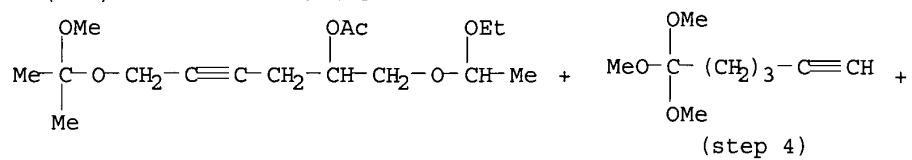


RX(213) OF 223 - 13 STEPS

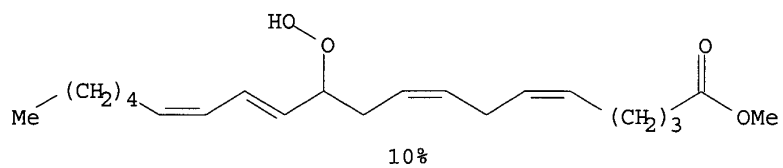
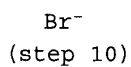




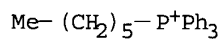
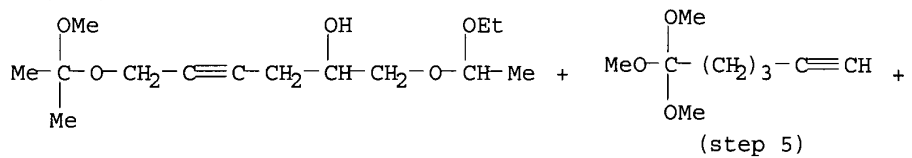
RX(217) OF 223 - 13 STEPS



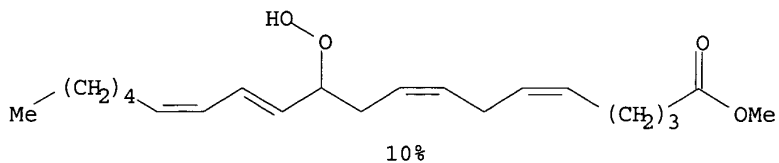
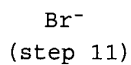
2. MeSO<sub>2</sub>Cl  
 9. Ph<sub>3</sub>P:CHCHO  
 12. MeSO<sub>2</sub>Cl



RX(219) OF 223 - 14 STEPS

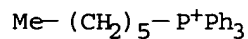
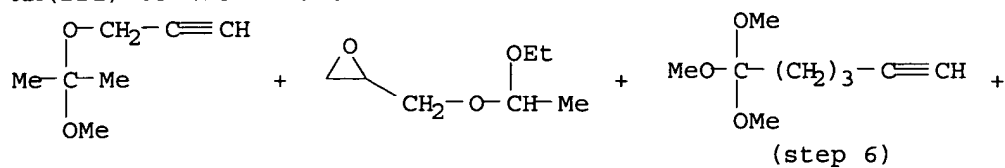
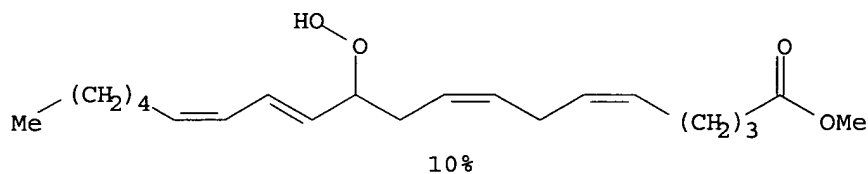
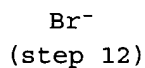


1. Ac<sub>2</sub>O  
 3. MeSO<sub>2</sub>Cl  
 10. Ph<sub>3</sub>P:CHCHO  
 13. MeSO<sub>2</sub>Cl

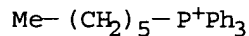
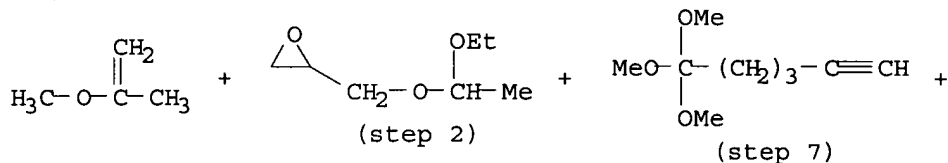




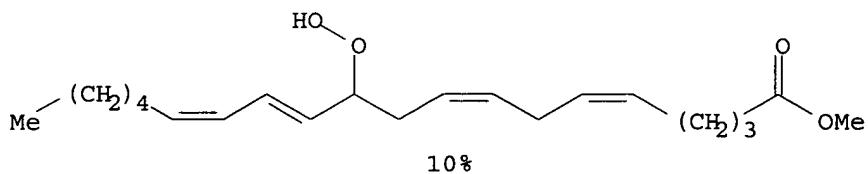
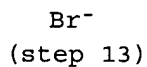
RX(221) OF 223 - 15 STEPS

2. Ac<sub>2</sub>O4. MeSO<sub>2</sub>Cl11. Ph<sub>3</sub>P:CHCHO14. MeSO<sub>2</sub>Cl

RX(223) OF 223 - 16 STEPS



1. Propargyl alcohol

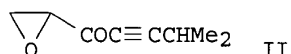
3. Ac<sub>2</sub>O5. MeSO<sub>2</sub>Cl12. Ph<sub>3</sub>P:CHCHO15. MeSO<sub>2</sub>Cl

L34 ANSWER 30 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 93:167543 CASREACT

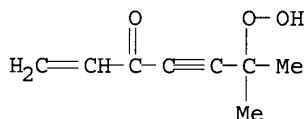
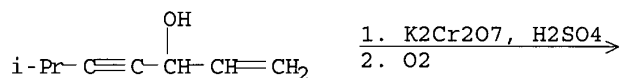
TITLE: Autoxidation of acetylenes. XXV. Products of the

AUTHOR(S): autooxidation of 2-methyl-6-hepten-3-yne  
 Kudrevatykh, M. V.; Tishchenko, I. G.; Chirko, A. I.  
 CORPORATE SOURCE: Beloruss. Gos. Univ., Minsk, USSR  
 SOURCE: Vestsi Akademii Navuk BSSR, Seryya Khimichnykh Navuk  
 (1980), (3), 110-14  
 CODEN: VBSKAK; ISSN: 0002-3590  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI

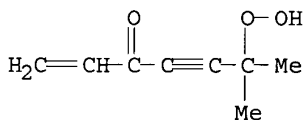
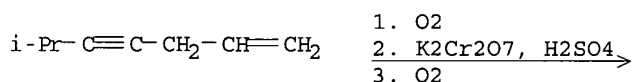


AB Grignard synthesis with  $\text{CH}_2\text{:CHCH}_2\text{Br}$  and  $\text{HC.tplbond.CCHMe}_2$  gave 80%  $\text{CH}_2\text{:CHCHXC:CCHMe}_2$  (I;  $\text{X} = \text{H}$ ), autoxidn. of which initially gave I ( $\text{X} = \text{OOH}$ ) and  $\text{CH}_2\text{:CHCH}_2\text{C.tplbond.CCMe}_2\text{OOH}$ . These decomposed to the corresponding alcs. Further oxidation of I ( $\text{X} = \text{OOH}$ ) yielded the ketone, which was oxidized still further to give  $\text{CH}_2\text{:CHCOC.tplbond.CCMe}_2\text{OOH}$  and epoxide II.

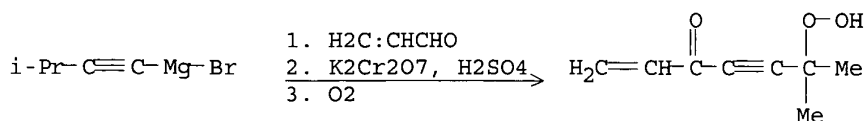
RX (21) OF 29 - 2 STEPS



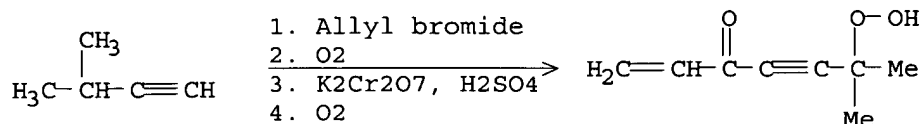
RX (25) OF 29 - 3 STEPS



RX (27) OF 29 - 3 STEPS



RX(29) OF 29 - 4 STEPS



=&gt; d l34 ibib abs hitstr 31-

YOU HAVE REQUESTED DATA FROM 46 ANSWERS - CONTINUE? Y/(N):y

L34 ANSWER 31 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:387846 CAPLUS

DOCUMENT NUMBER: 142:431972

TITLE: Process for the oxidation of cyclohexane

INVENTOR(S): Landray, David Paul; Fodor, Ludovic Rick; Murphree, Bruce Edwin; Rung, James Marvin

PATENT ASSIGNEE(S): Invista North America S.A.R.L., USA

SOURCE: U.S., 8 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6888034	B1	20050503	US 2003-702255	20031105
US 2005096486	A1	20050505		
WO 2005047243	A1	20050526	WO 2004-US36480	20041103

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-702255 A 20031105

OTHER SOURCE(S): CASREACT 142:431972

AB A process for oxidizing cyclohexane into cyclohexyl hydroperoxide, cyclohexanone, and cyclohexanol is described in which oxygen is contacted with cyclohexane at a pre-selected feed rate in a first reaction zone and unconsumed oxygen is contacted with cyclohexane in a second reaction zone in which the cyclohexane feed rate is lower than the pre-selected feed rate. Process flow diagrams are presented.

IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(in a process for the oxidation of cyclohexane)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

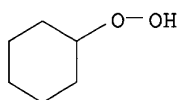
IT 7440-47-3, Chromium, processes 7440-48-4, Cobalt,  
processes  
RL: CAT (Catalyst use); EPR (Engineering process); PEP  
(Physical, engineering or chemical process); PROC (Process); USES (Uses)  
(oxidation catalyst; in a process for the oxidation of cyclohexane)  
RN 7440-47-3 CAPLUS  
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

RN 7440-48-4 CAPLUS  
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

IT 766-07-4P, Cyclohexyl hydroperoxide  
RL: EPR (Engineering process); IMF (Industrial manufacture); PEP  
(Physical, engineering or chemical process); PREP (Preparation);  
PROC (Process)  
(process for the oxidation of cyclohexane)  
RN 766-07-4 CAPLUS  
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)

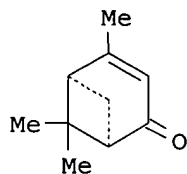


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

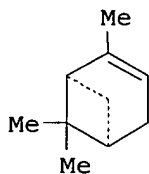
L34 ANSWER 32 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2005:341550 CAPLUS  
DOCUMENT NUMBER: 142:411505  
TITLE: Method for the preparation of verbenone from  
 $\alpha$ -pinene  
INVENTOR(S): Frolova, L. L.; Kuchin, A. V.; Dreval, I. V.;  
Panteleeva, M. V.; Alekseev, I. N.  
PATENT ASSIGNEE(S): Gosudarstvennoe Uchrezhdenie Institut Khimii Komi  
Nauchnogo Tsentra Ural'skogo Otdeleniya Rossiiskoi  
Akademii Nauk, Russia  
SOURCE: Russ., No pp. given  
CODEN: RUXXE7  
DOCUMENT TYPE: Patent

LANGUAGE: Russian  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RU 2250208	C2	20050420	RU 2003-121762	20030714
PRIORITY APPLN. INFO.:			RU 2003-121762	20030714
OTHER SOURCE(S):	CASREACT 142:411505; MARPAT 142:411505			
GI				



I



II

AB Invention provides a method for preparation of verbenone (I), which is important intermediate in synthesis of perfumes, optically active insect pheromones and therapeutical preps. Method involves catalytic oxidation of  $\alpha$ -pinene (II) with air oxygen, wherein catalysts are selected from: a group including bivalent Cu, Zn, Pb, Co, Mn, and Ni (preferably Co, Mn, Ni), and Cr(III); a pyridine complex,  $M(C_5H_5N)_2X_2$  [M represents bivalent transition metal, in particular, Co, Ni, and Mn; and X = halogen, e.g., Cl or Br]; or  $CrO_3 \cdot M(C_5H_5N)_2$ . Resulting hydroperoxides are then decomposed via fractioning steam distillation in alkali medium, wherein nonconverted  $\alpha$ -pinene is separated at temperature below 97°C, whereas oxidized product fraction is distilled at 97-100°C and then subjected to addnl. oxidation with chromic mixture followed by recovering verbenone from addnl. oxidized products. Verbenone is further freed from myrtenal ingredient by reducing it into myrtenol with alkali metal borohydride in alc. or water-alc. solution, after which verbenone is recovered from reduction products.

IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)

(oxidation by, of  $\alpha$ -pinene; preparation of verbenone from  $\alpha$ -pinene via catalytic air oxidation)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 14024-85-2 14024-92-1 14872-18-5

20492-50-6, Dipyridinechromium trioxide 162635-76-9, Chromium triseicosanoate

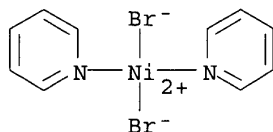
RL: CAT (Catalyst use); USES (Uses)

(oxidation catalyst; preparation of verbenone from  $\alpha$ -pinene via

catalytic air oxidation)

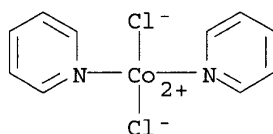
RN 14024-85-2 CAPLUS

CN Nickel, dibromobis(pyridine)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



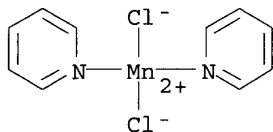
RN 14024-92-1 CAPLUS

CN Cobalt, dichlorobis(pyridine)-, (T-4)- (9CI) (CA INDEX NAME)



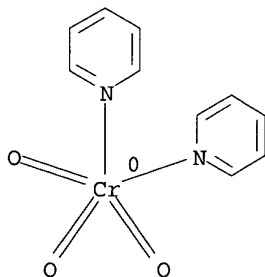
RN 14872-18-5 CAPLUS

CN Manganese, dichlorobis(pyridine)-, (T-4)- (9CI) (CA INDEX NAME)



RN 20492-50-6 CAPLUS

CN Chromium, trioxobis(pyridine)-, (TB-5-22)- (9CI) (CA INDEX NAME)



RN 162635-76-9 CAPLUS

CN Eicosanoic acid, chromium(3+) salt (9CI) (CA INDEX NAME)

$\text{HO}_2\text{C}^--(\text{CH}_2)_{18}-\text{Me}$

● 1/3 Cr(III)

IT 850428-67-0P

RL: RCT (Reactant); **SPN (Synthetic preparation); PREP**

**(Preparation)**; RACT (Reactant or reagent)

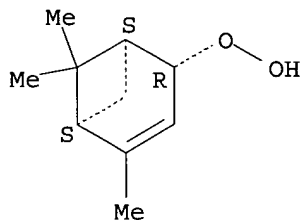
(preparation and decomposition of, via fractioning steam distillation;  
preparation of

verbenone from  $\alpha$ -pinene via catalytic air oxidation)

RN 850428-67-0 CAPLUS

CN Hydroperoxide, (1R,2S,5R)-4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl,  
rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



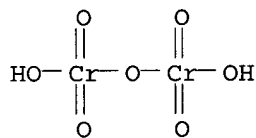
IT 13530-68-2D, Chromic acid, Jones reagent

RL: RGT (Reagent); RACT (Reactant or reagent)

(preparation of verbenone from  $\alpha$ -pinene via **catalytic** air oxidation)

RN 13530-68-2 CAPLUS

CN Chromic acid (H<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>) (9CI) (CA INDEX NAME)



L34 ANSWER 33 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:317672 CAPLUS

DOCUMENT NUMBER: 142:489452

TITLE: Double channel electrode flow cell application to the  
study of HO<sub>2</sub>- production on Mn<sub>x</sub>Co<sub>3-x</sub>O<sub>4</sub> (0 ≤ x  
≤ 1) spinel films

AUTHOR(S): Rios, E.; Reyes, H.; Ortiz, J.; Gautier, J. L.

CORPORATE SOURCE: Laboratorio de Electroquímica y Fisicoquímica de  
Sólidos, Departamento de Química de los Materiales,  
Facultad de Química y Biología, Universidad de  
Santiago de Chile, Santiago, 7254758, Chile

SOURCE: Electrochimica Acta (2005), 50(13), 2705-2711

CODEN: ELCAAV; ISSN: 0013-4686  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The authors conducted a study on the electroredn. of O<sub>2</sub> in alkaline solution at room temperature on pure thin oxide electrodes Mn<sub>x</sub>Co<sub>3-x</sub>O<sub>4</sub> (0 ≤ x ≤ 1) using the double channel electrode flow cell (DCEFC). The oxides were prepared at 150° and deposited by spray pyrolysis onto Ti substrates. The oxygen reduction reaction (orr) occurs through interactive and parallel pathways, and the ratio of O<sub>2</sub> mols. reduced to OH<sup>-</sup> ions with respect to those reduced to HO<sub>2</sub><sup>-</sup> ions depends on the oxide stoichiometry and on the applied overpotential. The formation of HO<sub>2</sub><sup>-</sup> increases when the Mn concentration increases. The results obtained for the orr show that the number of electrons transferred per O<sub>2</sub> mol. decreases from 3 to 2 and the ratio k<sub>1</sub>/k<sub>2</sub> (the rate consts. for direct reduction to OH<sup>-</sup> and indirect reduction to HO<sub>2</sub><sup>-</sup>) increases, resp., in the overpotential studied range (-0.05 to -0.6 V). The Mn<sup>3+</sup> ions placed in the B-sites of the spinel structure seem to be the active centers, where H<sub>2</sub>O<sub>2</sub> is formed.

IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (electrochem. reduction on Mn<sub>x</sub>Co<sub>3-x</sub>O<sub>4</sub> (0 ≤ x ≤ 1) spinel films in double channel electrode flow cell in HO<sub>2</sub><sup>-</sup> production)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 452976-56-6, Cobalt manganese oxide (Co<sub>2</sub>-3MnO-104)

RL: CAT (Catalyst use); DEV (Device component use); USES (Uses)  
 (oxygen electrochem. reduction on Mn<sub>x</sub>Co<sub>3-x</sub>O<sub>4</sub> (0 ≤ x ≤ 1) spinel films in double channel electrode flow cell in HO<sub>2</sub><sup>-</sup> production)

RN 452976-56-6 CAPLUS

CN Cobalt manganese oxide (Co<sub>2</sub>-3MnO-104) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====+=====+=====		
O	4	17778-80-2
Co	2 - 3	7440-48-4
Mn	0 - 1	7439-96-5

IT 14691-59-9P, Peroxide (HO<sub>2</sub><sup>-</sup>)

RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (oxygen electrochem. reduction on Mn<sub>x</sub>Co<sub>3-x</sub>O<sub>4</sub> (0 ≤ x ≤ 1) spinel films in double channel electrode flow cell in HO<sub>2</sub><sup>-</sup> production)

RN 14691-59-9 CAPLUS

CN Peroxide (HO<sub>2</sub><sup>-</sup>) (8CI, 9CI) (CA INDEX NAME)

-O-OH

IT 1308-06-1, Cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) 12139-92-3, Cobalt manganese oxide (Co<sub>2</sub>MnO<sub>4</sub>) 183864-63-3, Cobalt manganese oxide



(Co<sub>2.75</sub>Mn<sub>0.25</sub>O<sub>4</sub>) 183864-65-5, Cobalt manganese oxide

(Co<sub>2.5</sub>Mn<sub>0.5</sub>O<sub>4</sub>) 183864-67-7, Cobalt manganese oxide

(Co<sub>2.25</sub>Mn<sub>0.75</sub>O<sub>4</sub>)

RL: CAT (Catalyst use); DEV (Device component use); USES (Uses)

(oxygen electrochem. reduction on cobalt oxide and cobalt manganese oxide  
spinel films in double channel electrode flow cell in HO<sub>2</sub>- production)

RN 1308-06-1 CAPLUS

CN Cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 12139-92-3 CAPLUS

CN Cobalt manganese oxide (Co<sub>2</sub>MnO<sub>4</sub>) (6CI, 9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====	=====	=====
O	4	17778-80-2
Co	2	7440-48-4
Mn	1	7439-96-5

RN 183864-63-3 CAPLUS

CN Cobalt manganese oxide (Co<sub>2.75</sub>Mn<sub>0.25</sub>O<sub>4</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====	=====	=====
O	4	17778-80-2
Co	2.75	7440-48-4
Mn	0.25	7439-96-5

RN 183864-65-5 CAPLUS

CN Cobalt manganese oxide (Co<sub>2.5</sub>Mn<sub>0.5</sub>O<sub>4</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====	=====	=====
O	4	17778-80-2
Co	2.5	7440-48-4
Mn	0.5	7439-96-5

RN 183864-67-7 CAPLUS

CN Cobalt manganese oxide (Co<sub>2.25</sub>Mn<sub>0.75</sub>O<sub>4</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====	=====	=====
O	4	17778-80-2
Co	2.25	7440-48-4
Mn	0.75	7439-96-5

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 34 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:1052421 CAPLUS

DOCUMENT NUMBER: 142:155918

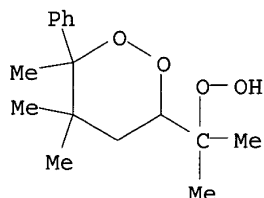
TITLE: Synthesis of Cyclic Peroxides by Chemo- and  
Regioselective Peroxidation of Dienes with  
Co(II)/O<sub>2</sub>/Et<sub>3</sub>SiH

AUTHOR(S): Tokuyasu, Takahiro; Kunikawa, Shigeki; McCullough, Kevin J.; Masuyama, Araki; Nojima, Masatomo  
 CORPORATE SOURCE: Department of Materials Chemistry, Frontier Research Center, Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan  
 SOURCE: Journal of Organic Chemistry (2005), 70(1), 251-260  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB In the competitive peroxidn. of mixts. of two alkenes with Co(II)/O<sub>2</sub>/Et<sub>3</sub>SiH, it was found that the relative reactivities of the alkene substrates are influenced by three major factors: relative stability of the intermediate carbon-centered radical formed by the reaction of the alkene with HCo(III) complex, steric effects around the carbon-carbon double bond, and electronic factors associated with the carbon-carbon double bond. Consistent with results from simple alkenes, the chemoselective and regioselective peroxidn. of dienes was also realized. Depending on the diene structure, the product included not only the expected acyclic unsatd. triethylsilyl peroxides but also 1,2-dioxolane and 1,2-dioxane derivs. via intramol. cyclization of the unsatd. peroxy radical intermediates.

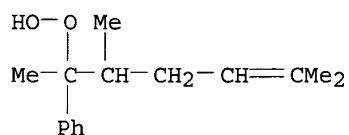
IT **830345-40-9P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of [(1,2-dioxanyl)methyl]hydroperoxide and study of its crystal and mol. structures)

RN 830345-40-9 CAPLUS  
 CN Hydroperoxide, 1-methyl-1-(5,5,6-trimethyl-6-phenyl-1,2-dioxan-3-yl)ethyl (9CI) (CA INDEX NAME)

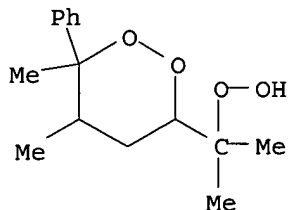


IT **830345-32-9P 830345-33-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of cyclic peroxides, dioxane derivs. and silyl peroxides by chemoselective, regioselective peroxidn. of [dimethyl(methylene)hexenyl]benzene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)

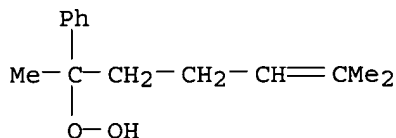
RN 830345-32-9 CAPLUS  
 CN Hydroperoxide, 1,2,5-trimethyl-1-phenyl-4-hexenyl (9CI) (CA INDEX NAME)



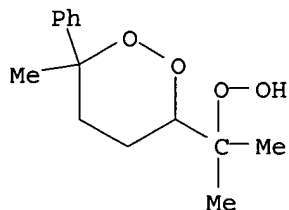
RN 830345-33-0 CAPLUS  
 CN Hydroperoxide, 1-(5,6-dimethyl-6-phenyl-1,2-dioxan-3-yl)-1-methylethyl  
 (9CI) (CA INDEX NAME)



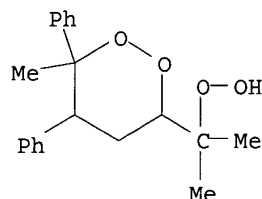
IT 830345-29-4P 830345-30-7P 830345-38-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of cyclic peroxides, dioxane derivs. and silyl peroxides by  
 chemoselective, regioselective peroxidn. of  
 [methyl(methylene)hexenyl]benzene using bis[[di(methyl)di(oxo-κO) -  
 (oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)  
 RN 830345-29-4 CAPLUS  
 CN Hydroperoxide, 1,5-dimethyl-1-phenyl-4-hexenyl (9CI) (CA INDEX NAME)



RN 830345-30-7 CAPLUS  
 CN Hydroperoxide, 1-methyl-1-(6-methyl-6-phenyl-1,2-dioxan-3-yl)ethyl (9CI)  
 (CA INDEX NAME)



RN 830345-38-5 CAPLUS  
 CN Hydroperoxide, 1-methyl-1-(6-methyl-5,6-diphenyl-1,2-dioxan-3-yl)ethyl  
 (9CI) (CA INDEX NAME)



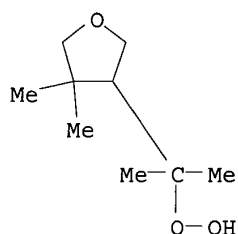
IT 830345-55-6P 830345-56-7P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(preparation of peroxide by chemoselective, regioselective peroxidn. of (methyl) [[ (methyl)propenyl]oxy]butene using bis[[di(methyl)di(oxo-κO) - (oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)

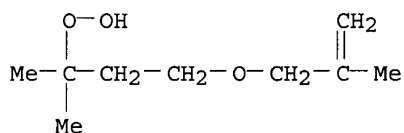
RN 830345-55-6 CAPLUS

CN Hydroperoxide, 1-methyl-1-(tetrahydro-4,4-dimethyl-3-furanyl)ethyl (9CI)  
(CA INDEX NAME)



RN 830345-56-7 CAPLUS

CN Hydroperoxide, 1,1-dimethyl-3-[(2-methyl-2-propenyl)oxy]propyl (9CI) (CA INDEX NAME)



IT 830345-51-2P

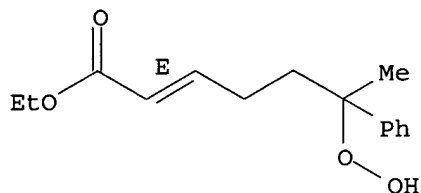
RL: **SPN (Synthetic preparation); PREP (Preparation)**

(preparation of peroxide by chemoselective, regioselective peroxidn. of (phenyl)heptadienoic acid ester using bis[[di(methyl)di(oxo-κO) - (oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)

RN 830345-51-2 CAPLUS

CN 2-Heptenoic acid, 6-hydroperoxy-6-phenyl-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



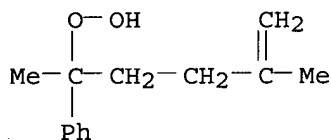
IT 830345-48-7P 830345-49-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of peroxide by chemoselective, regioselective peroxidn. of [(methyl) (methylene)pentenyl]benzene using bis[[di(methyl)di(oxo-κO) - (oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)

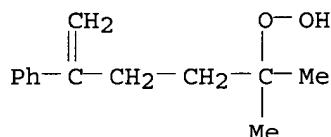
RN 830345-48-7 CAPLUS

CN Hydroperoxide, 1,4-dimethyl-1-phenyl-4-pentenyl (9CI) (CA INDEX NAME)



RN 830345-49-8 CAPLUS

CN Hydroperoxide, 1,1-dimethyl-4-phenyl-4-pentenyl (9CI) (CA INDEX NAME)



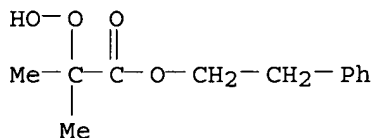
IT 830345-67-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of peroxide by chemoselective, regioselective peroxidn. of alkene using bis[[di(methyl)di(oxo-O) - (oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system and study of influence of electronic effects on product formation)

RN 830345-67-0 CAPLUS

CN Propanoic acid, 2-hydroperoxy-2-methyl-, 2-phenylethyl ester (9CI) (CA INDEX NAME)



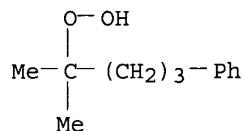
IT 34586-03-3P 42238-03-9P 42805-25-4P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(preparation of peroxide by chemoselective, regioselective peroxidn. of alkene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system and study of influence of steric congestion on product formation)

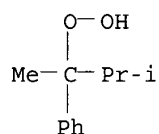
RN 34586-03-3 CAPLUS

CN Hydroperoxide, 1,1-dimethyl-4-phenylbutyl (9CI) (CA INDEX NAME)



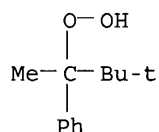
RN 42238-03-9 CAPLUS

CN Hydroperoxide, 1,2-dimethyl-1-phenylpropyl (9CI) (CA INDEX NAME)



RN 42805-25-4 CAPLUS

CN Hydroperoxide, 1,2,2-trimethyl-1-phenylpropyl (9CI) (CA INDEX NAME)



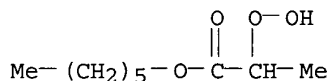
IT 830345-69-2P 830345-71-6P 830345-73-8P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(preparation of peroxide by peroxidn. of alkene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane and study of influence of relative stability of radical intermediates on product formation)

RN 830345-69-2 CAPLUS

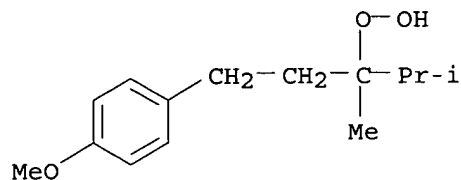
CN Propanoic acid, 2-hydroperoxy-, hexyl ester (9CI) (CA INDEX NAME)



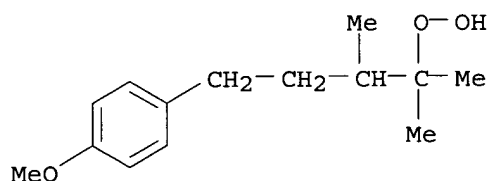
RN 830345-71-6 CAPLUS

CN Hydroperoxide, 1-[2-(4-methoxyphenyl)ethyl]-1,2-dimethylpropyl (9CI) (CA

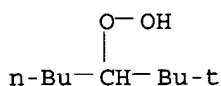
INDEX NAME)



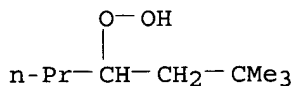
RN 830345-73-8 CAPLUS  
 CN Hydroperoxide, 4-(4-methoxyphenyl)-1,1,2-trimethylbutyl (9CI) (CA INDEX NAME)



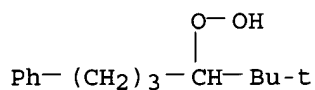
IT 830345-79-4P 830345-81-8P 830345-83-0P  
 830345-85-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of peroxide by peroxidn. of alkene using bis[[di(methyl)di(oxo-  
 κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system  
 and study of influence of relative reactivity on product formation)  
 RN 830345-79-4 CAPLUS  
 CN Hydroperoxide, 1-(1,1-dimethylethyl)pentyl (9CI) (CA INDEX NAME)



RN 830345-81-8 CAPLUS  
 CN Hydroperoxide, 3,3-dimethyl-1-propylbutyl (9CI) (CA INDEX NAME)

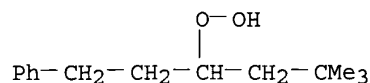


RN 830345-83-0 CAPLUS  
 CN Hydroperoxide, 1-(1,1-dimethylethyl)-4-phenylbutyl (9CI) (CA INDEX NAME)



RN 830345-85-2 CAPLUS

CN Hydroperoxide, 3,3-dimethyl-1-(2-phenylethyl)butyl (9CI) (CA INDEX NAME)



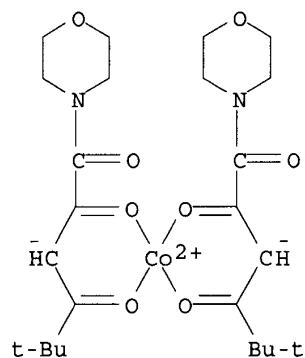
IT 124027-94-7, Bis(1-morpholinocarbamoyl-4,4-dimethyl-1,3-pentanedionato)cobalt(II)

RL: **CAT (Catalyst use)**; USES (Uses)

(preparation of peroxides by chemoselective, regioselective peroxidn. of dienes using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)

RN 124027-94-7 CAPLUS

CN Cobalt, bis[4-[5,5-dimethyl-2,4-di(oxo-κO)-1-oxohexyl]morpholinato]-(9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions

RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**

(preparation of peroxides by chemoselective, regioselective peroxidn. of dienes using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 830345-26-1P 830345-27-2P

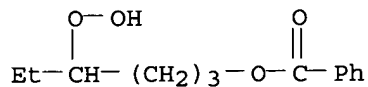
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(study of peroxidn. of (Z)-hexenol benzoate using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)

RN 830345-26-1 CAPLUS

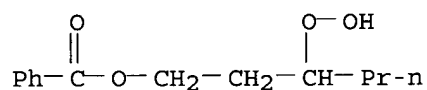
CN 1-Hexanol, 4-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)





RN 830345-27-2 CAPLUS

CN 1-Hexanol, 3-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)

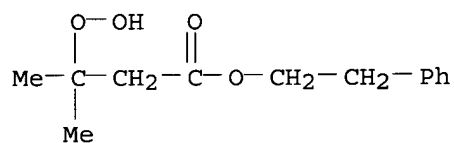


IT 830345-24-9P 830345-25-0P

RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (study of peroxidn. of (methyl)butenoic acid phenylethyl ester using  
 bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/t  
 riethylsilane-d system)

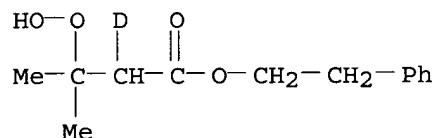
RN 830345-24-9 CAPLUS

CN Butanoic acid, 3-hydroperoxy-3-methyl-, 2-phenylethyl ester (9CI) (CA INDEX NAME)



RN 830345-25-0 CAPLUS

CN Butanoic-2-d acid, 3-hydroperoxy-3-methyl-, 2-phenylethyl ester (9CI) (CA INDEX NAME)

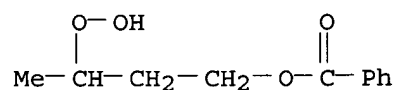


IT 830345-65-8P

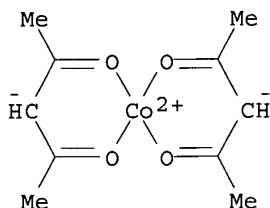
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (study of peroxidn. of butenol benzoate using  
 bis(pentanedionato)cobalt/oxygen/triethylsilane system)

RN 830345-65-8 CAPLUS

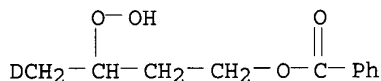
CN 1-Butanol, 3-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)



IT **14024-48-7**, Bis(acetylacetonato)cobalt  
 RL: **CAT (Catalyst use)**; **USES (Uses)**  
 (study of peroxidn. of butenol benzoate using  
 bis(pentanedionato)cobalt/oxygen/triethylsilane-d system)  
 RN 14024-48-7 CAPLUS  
 CN Cobalt, bis(2,4-pentanedionato- $\kappa$ O, $\kappa$ O')-, (SP-4-1)- (9CI) (CA  
 INDEX NAME)



IT **830345-28-3P**  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (study of peroxidn. of butenol benzoate using  
 bis(pentanedionato)cobalt/oxygen/triethylsilane-d system)  
 RN 830345-28-3 CAPLUS  
 CN 1-Butan-4-d-ol, 3-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 35 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:817834 CAPLUS

DOCUMENT NUMBER: 141:316241

TITLE: Process for the catalytic hydrogenation of alkylaryl  
 ketones in the presence of phenolic compounds

INVENTOR(S): Nisbet, Timothy Michael; Van Zwienen, Marinus

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004085354	A2	20041007	WO 2004-EP50362	20040325
WO 2004085354	A3	20050317		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,  
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,  
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,  
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,  
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,  
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,  
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,  
TD, TG

US 2004220431 A1 20041104 US 2004-808858 20040325  
PRIORITY APPLN. INFO.: EP 2003-251987 A 20030328  
AB A process for the catalytic hydrogenation of alkylaryl ketones (e.g., acetophenone) into their corresponding alcs. (e.g., 1-phenyl-1-ethanol) comprises contacting a feed comprising the alkylaryl ketones and 0.5-30% of phenolic compds. (e.g., phenol) with hydrogen in the presence of a heterogeneous hydrogenation catalyst (e.g., copper). A process for preparing a hydrogenation catalyst with improved activity, and to the use of phenolic compds. for the activation of the hydrogenation catalysts is described.  
IT 7782-44-7, Oxygen, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of alkylaryl compds. with)  
RN 7782-44-7 CAPLUS  
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

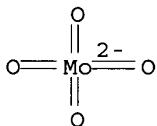
O=O

IT 7440-50-8, Copper, uses  
RL: CAT (Catalyst use); USES (Uses)  
(process for the catalytic hydrogenation of alkylaryl ketones in the presence of phenolic compds.)  
RN 7440-50-8 CAPLUS  
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

L34 ANSWER 36 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2004:261000 CAPLUS  
DOCUMENT NUMBER: 140:287556  
TITLE: Process for singlet oxygen oxidation of organic substrates  
INVENTOR(S): Emsenhuber, Martin; Kwant, Gerard; Van Straaten, Koenraad; Janssen, Madelon; Alsters, Paul; Hoving, Hendrik  
PATENT ASSIGNEE(S): DSM Fine Chemicals Austria Nfg G.m.b.H. & Co. K.-G., Austria  
SOURCE: Eur. Pat. Appl., 10 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1403234	A2	20040331	EP 2003-19797	20030830
EP 1403234	A3	20040519		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AT 200201443	A5	20050415	AT 2002-1443	20020926
US 2004220416	A1	20041104	US 2003-668259	20030924
JP 2004137269	A2	20040513	JP 2003-334055	20030925
PRIORITY APPLN. INFO.:			AT 2002-1443	A 20020926
OTHER SOURCE(S): CASREACT 140:287556				
AB Improved procedure for the oxidation of organic substrates, especially olefins				
[1 - 10				
double bonds, (un)substituted C6-30-aroms., polyaroms. (2 - 8 rings), alkylsulfides, alkenylsulfides, arylsulfides, C4-30-heterocyclics (with 1 or more O, N, S); substituted with halogen, CN, :CO, OH, C1-20-alkoxy, C1-20-alkyl, C6-30-aryl, C2-20-alkenyl, C2-20-alkynyl, CO2H, ester, amide, NH2, NO2, silyl, siloxy, sulfono, sulfoxo, NR1R2; R1, R2 = H, C1-20-alkyl, CHO, C2-20-acyl, C7-30-benzoyl; R1R2 = ring], with singlet oxygen is characterized by reaction of the organic substrate with 1O2 in H2O or an aqueous solution of a water miscible organic solvent in the presence of a heterogeneous or homogeneous catalyst and aqueous H2O2 whereby the catalyst decomposes the H2O2 to 1O2 and water is removed from the reaction by a water selective membrane. Thus, $\beta$ -citronellol in an aqueous methanol solution containing catalytic Na2MoO4 is treated with aqueous H2O2 whereby the solution is pumped past a membrane separating out the H2O. Water removal with a pervaporation membrane was tested with a test solution containing sodium tiglate in aqueous MeOH.				
Process schematics are provided.				
IT 7631-95-0, Sodium molybdate				
RL: CAT (Catalyst use); USES (Uses)				
(decomposition catalyst; process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by a water selective membrane)				
RN 7631-95-0 CAPLUS				
CN Molybdate (MoO42-), disodium, (T-4)- (9CI) (CA INDEX NAME)				



● 2 Na<sup>+</sup>

IT 7439-98-7D, Molybdenum, compds. 7440-62-2D, Vanadium, compds.

RL: CAT (Catalyst use); USES (Uses)

(decomposition catalysts; process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by a water selective membrane)

RN 7439-98-7 CAPLUS

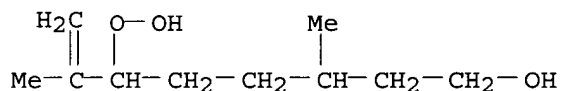
CN Molybdenum (8CI, 9CI) (CA INDEX NAME)

Mo

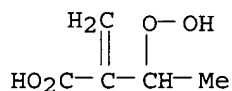
RN 7440-62-2 CAPLUS  
 CN Vanadium (8CI, 9CI) (CA INDEX NAME)

V

IT 81113-74-8P 99268-55-0P  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by a water selective membrane)  
 RN 81113-74-8 CAPLUS  
 CN 7-Octen-1-ol, 6-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 99268-55-0 CAPLUS  
 CN Butanoic acid, 3-hydroperoxy-2-methylene- (9CI) (CA INDEX NAME)



IT 7782-44-7D, Oxygen, singlet  
 RL: **RCT (Reactant); RACT (Reactant or reagent)**  
 (reaction of, with citronellol and tiglate; process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by a water selective membrane)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

L34 ANSWER 37 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:431670 CAPLUS  
 DOCUMENT NUMBER: 141:125349  
 TITLE: Uncatalyzed Liquid-Phase Oxidation of Cyclododecene with Molecular Oxygen  
 AUTHOR(S): Mahajan, S. S.; Sharma, M. M.; Sridhar, T.

CORPORATE SOURCE: Department of Chemical Engineering, Monash University,  
Victoria, 3800, Australia  
SOURCE: Industrial & Engineering Chemistry Research (2004),  
43(13), 3289-3296  
CODEN: IECRED; ISSN: 0888-5885  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 141:125349

AB Uncatalyzed liquid-phase oxidation of cyclododecene was studied in a batch reactor. Cyclododecene was oxidized with mol. oxygen at of 363-383 K. Cyclododecene oxide, cyclododecene hydroperoxide, and cyclododecenol were obtained as reaction products. The oxidation kinetics were studied in detail, and a mechanism was devised based on the exptl. results and existing literature. The kinetic data were generated at different reaction parameters and fitted successfully with a rate equation based on autocatalysis by total products. The values of the reaction rate consts. and activation energy were determined. A distinct difference was observed between the reaction rates of the cis and trans isomers of cyclododecene. The oxidation kinetics were also studied in a stainless steel reactor to examine the catalytic effect on reactivity of cyclododecene; no difference was observed vs. glass wall reactors. The presence of metal ions was found to affect the product distribution.

IT **7782-44-7**, Oxygen, reactions  
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**  
(kinetics and mechanism of uncatalyzed liquid-phase oxidation of cyclododecene with mol. oxygen)

RN 7782-44-7 CAPLUS

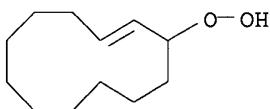
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT **723308-17-6P**, Cyclododecene hydroperoxide  
RL: **IMF (Industrial manufacture)**; **PREP (Preparation)**  
(kinetics and mechanism of uncatalyzed liquid-phase oxidation of cyclododecene with mol. oxygen)

RN 723308-17-6 CAPLUS

CN Hydroperoxide, 2-cyclododecen-1-yl (9CI) (CA INDEX NAME)



IT **11107-04-3**, SS 316  
RL: DEV (Device component use); USES (Uses)  
(reactor; kinetics and mechanism of **uncatalyzed** liquid-phase oxidation of cyclododecene with mol. oxygen)

RN 11107-04-3 CAPLUS

CN Iron alloy, base, Fe 62-72,Cr 16.00-18.00,Ni 10.00-14.00,Mn 2.00-3.00,Mn

0-2.00,Si 0-1.00,C 0-0.08,P 0-0.045,S 0-0.030 (UNS S31600) (9CI) (CA INDEX NAME)

Component	Component Percent	Component Registry Number
Fe	62 - 72	7439-89-6
Cr	16.00 - 18.00	7440-47-3
Ni	10.00 - 14.00	7440-02-0
Mo	2.00 - 3.00	7439-98-7
Mn	0 - 2.00	7439-96-5
Si	0 - 1.00	7440-21-3
C	0 - 0.08	7440-44-0
P	0 - 0.045	7723-14-0
S	0 - 0.030	7704-34-9

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 38 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:166974 CAPLUS

DOCUMENT NUMBER: 138:221456

TITLE: Preparation of olefin oxidation products using heteropoly acid catalysts

INVENTOR(S): Furuya, Masahiko; Nakashima, Hitoshi

PATENT ASSIGNEE(S): Asahi Kasei Corporation, Japan; Noguchi Research Institute

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003064007	A2	20030305	JP 2001-258538	20010828
PRIORITY APPLN. INFO.:			JP 2001-258538	20010828

AB The products are prepared by oxidation of olefins by mol. O in the presence of heteropoly acid catalysts containing rare earth elements, Group IVB, VB, VIB, or VIIB elements, Ni, Pd, Ir, or Pt in their double defects. Cyclooctene was oxidized by O in dichloroethane-MeCN mixture in the presence of Y-substituted tetrabutylammonium tungstosilicate (preparation given) at 75° for 75 h to give cyclooctene oxide with 86% selectivity at 20% conversion.

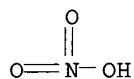
IT 13138-45-9DP, Nickel dinitrate, reaction products with decatungstosilicic acid and tetrabutylammonium nitrate

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(catalyst; preparation of olefin oxidation products using heteropoly acid catalysts)

RN 13138-45-9 CAPLUS

CN Nitric acid, nickel(2+) salt (8CI, 9CI) (CA INDEX NAME)

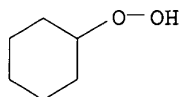


● 1/2 Ni(II)

IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (mol.; preparation of olefin oxidation products using heteropoly acid catalysts)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 27254-23-5P, Cyclohexenyl hydroperoxide  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of olefin oxidation products using heteropoly acid catalysts)  
 RN 27254-23-5 CAPLUS  
 CN Hydroperoxide, cyclohexenyl (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 766-07-4  
 CMF C6 H12 O2



L34 ANSWER 39 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:791395 CAPLUS  
 DOCUMENT NUMBER: 139:291994  
 TITLE: Method and cobalt-ruthenium catalyst systems for oxidizing cycloalkanes into cycloalkanols and cycloalkanones and hydroperoxycycloalkanes  
 INVENTOR(S): Tani, Nobuhiro; Murata, Shuzo  
 PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan  
 SOURCE: Eur. Pat. Appl., 8 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 EP 1350783 A1 20031008 EP 2003-7537 20030401  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 JP 2004002327 A2 20040108 JP 2003-77387 20030320  
 US 2003216601 A1 20031120 US 2003-396832 20030326  
 CN 1448378 A 20031015 CN 2003-121238 20030328  
 PRIORITY APPLN. INFO.: JP 2002-101001 A 20020403  
 OTHER SOURCE(S): CASREACT 139:291994  
 AB A method for producing an oxygenated compound (e.g., cyclohexanol and mixts.  
 of cyclohexanone and cyclohexyl hydroperoxide) from a cycloalkane (e.g.,  
 cyclohexane) is characterized in that the cycloalkane is contacted with  
 oxygen in the presence of a cobalt compound [e.g., cobalt(II) octylate] and  
 a ruthenium compound [e.g., ruthenium(III) acetylacetonate].  
 IT **1588-79-0**, CobaltII octanoate **7440-48-4**, Cobalt, uses  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (method and cobalt-ruthenium **catalyst** systems for oxidizing  
 cycloalkanes into cycloalkanols and cycloalkanones and  
 hydroperoxycycloalkanes)  
 RN 1588-79-0 CAPLUS  
 CN Octanoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)

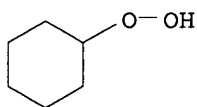
HO<sub>2</sub>C- (CH<sub>2</sub>)<sub>6</sub>-Me

● 1/2 Co(II)

RN 7440-48-4 CAPLUS  
 CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

IT **766-07-4P**, Cyclohexyl hydroperoxide  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (method and cobalt-ruthenium catalyst systems for oxidizing  
 cycloalkanes into cycloalkanols and cycloalkanones and  
 hydroperoxycycloalkanes)  
 RN 766-07-4 CAPLUS  
 CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions  
 RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**  
 (method and cobalt-ruthenium catalyst systems for oxidizing  
 cycloalkanes into cycloalkanols and cycloalkanones and

hydroperoxycycloalkanes using)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 40 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:458023 CAPLUS  
 DOCUMENT NUMBER: 142:96308  
 TITLE: Method for preparing cyclohexanone and cyclohexanol from cyclohexane  
 INVENTOR(S): Zhou, Xiaowen; Liu, Jihong; Yin, Huaqing; Hu, Xuewu; Li, Juan  
 PATENT ASSIGNEE(S): Yueyang Petro-Chemical General Plant, Baling Petro-Chemical Co., Peop. Rep. China  
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11 pp. CODEN: CNXXEV  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Chinese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

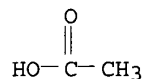
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1397538	A	20030219	CN 2001-114586	20010713

PRIORITY APPLN. INFO.: CN 2001-114586 20010713

AB A method comprises oxidizing cyclohexane with an O-containing gas to obtain cyclohexyl hydroperoxide-containing mixts., decomposing with aqueous Na<sub>2</sub>CO<sub>3</sub> solns. optionally containing Na carboxylates in the presence of 0.1-100 ppm soluble transition metal salt (such as Co sulfate or Co acetate) catalysts at 60°-120° and 100-1,200 kPa, decomposing again with aqueous NaOH solns. optionally containing Na carboxylates in the presence of 0.1-10 ppm soluble transition metal salts at 100-1,200 kPa, and distilling

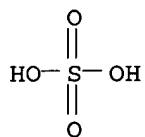
IT 5931-89-5, Cobalt acetate 10124-43-3, Cobalt sulfate  
 RL: CAT (Catalyst use); USES (Uses)  
 (oxidation of cyclohexane for manufacture of cyclohexanone and cyclohexanol)

RN 5931-89-5 CAPLUS  
 CN Acetic acid, cobalt salt (8CI, 9CI) (CA INDEX NAME)



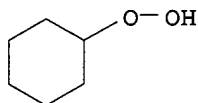
●<sub>x</sub> Co(x)

RN 10124-43-3 CAPLUS  
 CN Sulfuric acid, cobalt(2+) salt (1:1) (8CI, 9CI) (CA INDEX NAME)



● Co(II)

IT 766-07-4P, Cyclohexyl hydroperoxide  
 RL: **IMF (Industrial manufacture)**; RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)  
 (oxidation of cyclohexane for manufacture of cyclohexanone and cyclohexanol)  
 RN 766-07-4 CAPLUS  
 CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)

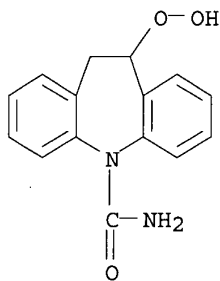


IT 7782-44-7, Oxygen, reactions  
 RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**  
 (oxidation of cyclohexane for manufacture of cyclohexanone and cyclohexanol)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

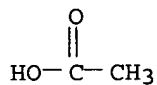


L34 ANSWER 41 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:109222 CAPLUS  
 DOCUMENT NUMBER: 139:22104  
 TITLE: Low temperature, high conversion, liquid-phase  
 benzylic oxidation with dioxygen by  
 metal/NHPI-catalyzed Co-oxidation with benzaldehyde  
 AUTHOR(S): Schmieder-van de Vondervoort, Lizette; Bouttemy,  
 Sabine; Heu, Ferdinand; Weissenbock, Kurt; Alsters,  
 Paul L.  
 CORPORATE SOURCE: Advanced Synthesis and Catalysis, DSM Fine Chemicals,  
 Geleen, 6160 MD, Neth.  
 SOURCE: European Journal of Organic Chemistry (2003), (3),  
 578-586  
 CODEN: EJOCFK; ISSN: 1434-193X  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:22104

- AB A new liquid-phase catalytic oxidation system for the low temperature, high conversion benzylic mono-oxyfunctionalization of 5H-dibenz[b,f]azepine-5-carboxamide (I) into oxcarbazepine with dioxygen has been developed. The method is based on a co-oxidation of I with benzaldehyde in the presence of a four-component catalyst system consisting of Co(OAc)<sub>2</sub>, Ni(OAc)<sub>2</sub>, Cr(NO<sub>3</sub>)<sub>3</sub>, and N-hydroxyphthalimide (NHPI). The influence of the catalyst system on the formation and decomposition of the crucial hydroperoxide intermediate has been investigated. Based on these results, the role of each of the components in the catalyst system is discussed. The scope of this method for the oxidation of other substrates has been studied, and the results are compared with those obtained by Co/NHPI catalyzed oxidation of these substrates.
- IT **537693-28-0P**, 10,11-Dihydro-10-hydroperoxy-5H-dibenz[b,f]azepine-5-carboxamide  
 RL: **BYP (Byproduct)**; RCT (Reactant); **PREP (Preparation)**  
 ; RACT (Reactant or reagent)  
 (low temperature, high-conversion, liquid-phase oxidation of  
 5H-dibenz[b,f]azepine-  
 5-carboxamide with dioxygen in presence of metal/N-hydroxyphthalimide  
 catalyst and benzaldehyde)
- RN 537693-28-0 CAPLUS
- CN 5H-Dibenz[b,f]azepine-5-carboxamide, 10,11-dihydro-10-hydroperoxy- (9CI)  
 (CA INDEX NAME)



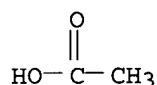
- IT **71-48-7**, Acetic acid cobalt(2+) salt **142-71-2**, Acetic acid copper(2+) salt **373-02-4**, Acetic acid nickel(2+) salt **638-38-0**, Acetic acid manganese(2+) salt **1313-27-5**, Molybdenum oxide (MoO<sub>3</sub>), uses **3094-87-9**, Acetic acid iron(2+) salt **3264-82-2**, Bis(acetylacetonato)nickel **7718-54-9**, Nickel chloride (NiCl<sub>2</sub>), uses **13476-99-8**, Tris(acetylacetonato)vanadium **13548-38-4**, Chromium nitrate [Cr(NO<sub>3</sub>)<sub>3</sub>] **21679-31-2**, Tris(acetylacetonato)chromium  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (low temperature, high-conversion, liquid-phase oxidation of benzylic  
 compds. with  
 dioxygen in presence of metal/N-hydroxyphthalimide **catalyst**  
 and benzaldehyde)
- RN 71-48-7 CAPLUS
- CN Acetic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

RN 142-71-2 CAPLUS

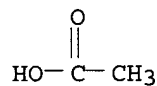
CN Acetic acid, copper(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Cu(II)

RN 373-02-4 CAPLUS

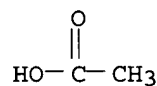
CN Acetic acid, nickel(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Ni(II)

RN 638-38-0 CAPLUS

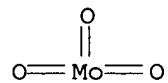
CN Acetic acid, manganese(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Mn(II)

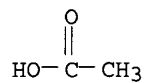
RN 1313-27-5 CAPLUS

CN Molybdenum oxide (MoO<sub>3</sub>) (7CI, 8CI, 9CI) (CA INDEX NAME)



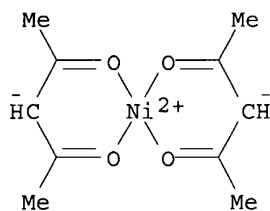
RN 3094-87-9 CAPLUS

CN Acetic acid, iron(2+) salt (8CI, 9CI) (CA INDEX NAME)

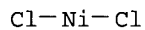


● 1/2 Fe(II)

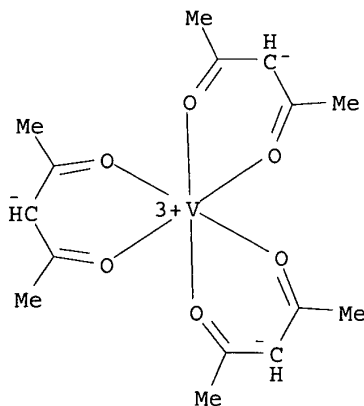
RN 3264-82-2 CAPLUS

CN Nickel, bis(2,4-pentanedionato- $\kappa\text{O},\kappa\text{O}'$ )-, (SP-4-1)- (9CI) (CA INDEX NAME)

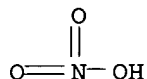
RN 7718-54-9 CAPLUS

CN Nickel chloride ( $\text{NiCl}_2$ ) (8CI, 9CI) (CA INDEX NAME)

RN 13476-99-8 CAPLUS

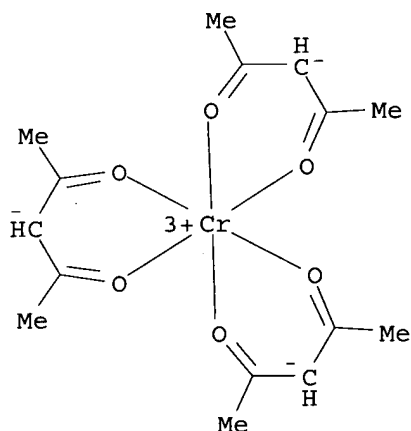
CN Vanadium, tris(2,4-pentanedionato- $\kappa\text{O},\kappa\text{O}'$ )-, (OC-6-11)- (9CI) (CA INDEX NAME)

RN 13548-38-4 CAPLUS  
 CN Nitric acid, chromium(3+) salt (8CI, 9CI) (CA INDEX NAME)



● 1/3 Cr(III)

RN 21679-31-2 CAPLUS  
 CN Chromium, tris(2,4-pentanedionato- $\kappa\text{O},\kappa\text{O}'$ )-, (OC-6-11)- (9CI)  
 (CA INDEX NAME)



IT 7782-44-7, Dioxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (low temperature, high-conversion, liquid-phase oxidation of benzylic  
 compds. with  
 dioxygen in presence of metal/N-hydroxyphthalimide catalyst and  
 benzaldehyde)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 42 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:290164 CAPLUS  
 DOCUMENT NUMBER: 139:133158  
 TITLE: Selective Oxidation of Ethylbenzene by Molecular

Oxygen: Effect of Macrocyclic 18-Crown-6 Polyether Additives on Catalysis by Bicyclic Nickel Complexes

AUTHOR(S): Matienko, L. I.; Mosolova, L. A.

CORPORATE SOURCE: Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, 119991, Russia

SOURCE: Kinetics and Catalysis (Translation of Kinetika i Kataliz) (2003), 44(2), 221-228  
CODEN: KICAA8; ISSN: 0023-1584

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

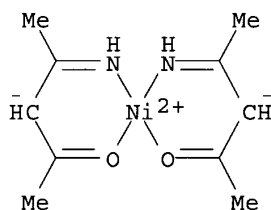
OTHER SOURCE(S): CASREACT 139:133158

AB The catalytic activity of the two-component catalytic system based on nickel bis(enaminoacetate) (enamac) and 18-crown-6 (18C6) macrocyclic polyether is studied in ethylbenzene oxidation by mol. oxygen. The {Ni(enamac)<sub>2</sub> & 18-crown-6} system is a more active catalyst of ethylbenzene oxidation into α-phenylethyl hydroperoxide compared to Ni(enamac)<sub>2</sub> and the {Ni(acac)<sub>2</sub> & 18-crown-6} system. The formation of Ni(enamac)<sub>2</sub>-18-crown-6 complex is confirmed both kinetically and spectroscopically. It is suggested that a rise in the oxidation selectivity is due to Ni(enamac)<sub>2</sub> transformation activated by 18-crown-6. The order of oxidation product formation at different oxidation stages is determined. The activity of catalysts in the elementary steps of the chain process is discussed.

IT 15170-64-6  
RL: CAT (Catalyst use); USES (Uses)  
(effect of macrocyclic crown polyether additives on catalysis by bicyclic nickel complexes)

RN 15170-64-6 CAPLUS

CN Nickel, bis[4-(imino-κN)-2-pentanonato-κO]- (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions  
RL: RGT (Reagent); RACT (Reactant or reagent)  
(effect of macrocyclic crown polyether additives on catalysis by bicyclic nickel complexes)

RN 7782-44-7 CAPLUS

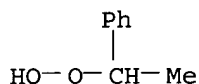
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 3071-32-7P, α-Phenylethyl hydroperoxide  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(effect of macrocyclic crown polyether additives on catalysis by



bicyclic nickel complexes)  
 RN 3071-32-7 CAPLUS  
 CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 43 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:450363 CAPLUS

DOCUMENT NUMBER: 137:33200

TITLE: Preparation of oxiranes by the epoxidation of alkenes with aralkyl hydroperoxides and regeneration of the hydroperoxides

INVENTOR(S): Vaporciyan, Garo Garbis; Murray, Brendan Dermot

PATENT ASSIGNEE(S): Shell Oil Company, Neth.

SOURCE: U.S. Pat. Appl. Publ., 4 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002072622	A1	20020613	US 2000-736522	20001213
US 6455712	B2	20020924		
WO 2002048125	A2	20020620	WO 2001-EP14748	20011213
WO 2002048125	A3	20030410		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
WO 2002048126	A2	20020620	WO 2001-EP14750	20011213
WO 2002048126	A3	20030417		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
WO 2002048127	A2	20020620	WO 2001-EP14751	20011213
WO 2002048127	A3	20030424		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, UZ, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,  
 GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,  
 GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002016112	A5	20020624	AU 2002-16112	20011213
AU 2002017114	A5	20020624	AU 2002-17114	20011213
AU 2002038433	A5	20020624	AU 2002-38433	20011213
EP 1343776	A2	20030917	EP 2001-986878	20011213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EP 1347962	A2	20031001	EP 2001-270532	20011213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EP 1366031	A2	20031203	EP 2001-270533	20011213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001016099	A	20031223	BR 2001-16099	20011213
BR 2001016100	A	20031223	BR 2001-16100	20011213
BR 2001016101	A	20031223	BR 2001-16101	20011213
JP 2004517841	T2	20040617	JP 2002-549656	20011213
JP 2004517842	T2	20040617	JP 2002-549657	20011213
TW 593298	B	20040621	TW 2001-90130928	20011213
JP 2004525870	T2	20040826	JP 2002-549658	20011213

PRIORITY APPLN. INFO.:

US 2000-736522	A	20001213
WO 2001-EP14748	W	20011213
WO 2001-EP14750	W	20011213
WO 2001-EP14751	W	20011213

OTHER SOURCE(S): CASREACT 137:33200

AB A process for preparing epoxides, which process comprises: (i) oxidizing an alkylaryl (e.g., cumene) to obtain a stream comprising alkylaryl hydroperoxide (e.g., cumene hydroperoxide); (ii) contacting at least a part of the alkylaryl hydroperoxide obtained in step (i) with an olefin (e.g., 1-octene) in the presence of a catalyst (e.g., Ti/SiO<sub>2</sub>) to obtain a product stream comprising an oxirane compound (e.g., n-hexyloxirane) and an alkylaryl hydroxyl compound (e.g., 2-phenyl-2-propanol); (iii) optionally reacting part of the alkylaryl hydroperoxide obtained in step (i) to obtain a mixture comprising (a) phenol, and (b) a ketone and/or aldehyde, and (c) optionally byproducts; (iv) separating the oxirane compound from the product

stream of step (ii) to obtain (a) a residual product stream and (b) oxirane, and (v) contacting at least a part of the residual product stream with hydrogen (i.e., hydrogenolysis) to obtain the alkylaryl compound, wherein at least a part of said alkylaryl is recycled to step (i).

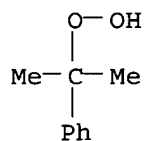
IT 80-15-9P, Cumene hydroperoxide 3071-32-7P, Ethylbenzene hydroperoxide

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

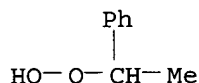
(epoxidizing agent; preparation of oxiranes by the epoxidn. of alkenes with aralkyl hydroperoxides and regeneration of the hydroperoxides)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



RN 3071-32-7 CAPLUS  
 CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



IT 7440-50-8, Copper, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (hydrogenolysis catalysts in a preparation of oxiranes by the  
 epoxidn. of alkenes with aralkyl hydroperoxides and regeneration of the  
 hydroperoxides using)  
 RN 7440-50-8 CAPLUS  
 CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of oxiranes by the epoxidn. of alkenes with aralkyl  
 hydroperoxides and regeneration of the hydroperoxides)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 44 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:672190 CAPLUS  
 DOCUMENT NUMBER: 137:203018  
 TITLE: Process for oxidation of organic substrates  
 INVENTOR(S): Tani, Nobuhiro; Murata, Shuzo  
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Daicel Chemical  
 Industries, Ltd.  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

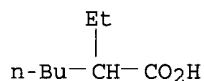
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002249451	A2	20020906	JP 2001-46389	20010222
PRIORITY APPLN. INFO.:			JP 2001-46389	20010222

AB The title process comprises contacting an organic substrate with oxygen in the presence of N-hydroxy cyclic imide,  $\leq 0.1$  mol% cobalt compound (relative to substrate), and  $\leq 0.1$  mol% vanadium compound (relative to substrate). Cyclohexane was oxidized by the title process to give cyclohexanone, cyclohexanol, cyclohexyl hydroperoxide, and adipic acid in 7.6%, 0.06%, 2.5%, and 1.3% yields, resp.

IT 136-52-7, Cobalt octoate  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (process for oxidation of organic substrates)

RN 136-52-7 CAPLUS

CN Hexanoic acid, 2-ethyl-, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)

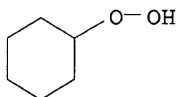


● 1/2 Co(II)

IT 766-07-4P, Cyclohexyl hydroperoxide  
 RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (process for oxidation of organic substrates)

RN 766-07-4 CAPLUS

CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions  
 RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**  
 (process for oxidation of organic substrates in presence of cobalt octanoate and vanadium naphthenate as catalysts)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 45 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:672188 CAPLUS  
 DOCUMENT NUMBER: 137:201098  
 TITLE: Continuous oxidation of organic substrates with

molecular oxygen and with high efficiency, and manufacture of oxygen-containing compounds by the method

INVENTOR(S): Murata, Shuzo; Tani, Nobuhiro  
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Daicel Chemical Industries, Ltd.  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002249450	A2	20020906	JP 2001-44752	20010221
PRIORITY APPLN. INFO.:			JP 2001-44752	20010221
OTHER SOURCE(S):	CASREACT 137:201098			

AB Organic substrates are continuously oxidized with supplying mixts. of the substrates, N-hydroxylated cyclic imides, and O-containing gas to solns. containing the imides whose concentration is higher than that of the imides in the

supplying mixts. Thus, air, a mixture of cyclohexane (I) and Co octylate (II), and a mixture of I, 0.25 weight% N-hydroxyphthalimide (III), and cyclohexanol (IV) were continuously supplied to a mixture of I, 0.5 weight% III, II, and IV over 5 h with retention time 1 h to give 0.5% adipic acid, and cyclohexanone, IV, and cyclohexyl hydroperoxide with 3.5% combined yield.

IT 6700-85-2

RL: **CAT (Catalyst use)**; USES (Uses)

(continuous oxidation of organic substrates with mol. oxygen in presence of transition metal **catalysts** and N-hydroxylated cyclic imides)

RN 6700-85-2 CAPLUS

CN Octanoic acid, cobalt salt (8CI, 9CI) (CA INDEX NAME)

$\text{HO}_2\text{C}-(\text{CH}_2)_6-\text{Me}$

●<sub>x</sub> Co(x)

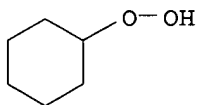
IT 766-07-4P, Cyclohexyl hydroperoxide

RL: **IMF (Industrial manufacture)**; **PREP (Preparation)**

(continuous oxidation of organic substrates with mol. oxygen in presence of transition metal catalysts and N-hydroxylated cyclic imides)

RN 766-07-4 CAPLUS

CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions  
 RL: **RCT (Reactant); RACT (Reactant or reagent)**  
 (continuous oxidation of organic substrates with mol. oxygen in presence of  
 transition metal catalysts and N-hydroxylated cyclic imides)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

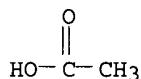
L34 ANSWER 46 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:514248 CAPLUS  
 DOCUMENT NUMBER: 137:63038  
 TITLE: Oxidation of organic compounds without decompositions  
 of imides  
 INVENTOR(S): Tani, Nobuhiro; Murata, Shuzo  
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Daicel Chemical  
 Industries, Ltd.  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002193855	A2	20020710	JP 2000-395772	20001226
PRIORITY APPLN. INFO.:			JP 2000-395772	20001226

OTHER SOURCE(S): CASREACT 137:63038

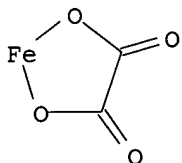
AB Organic substrates are oxidized by O in the presence of N-hydroxy cyclic imides and  $\leq 0.1$  mol% (to substrates)  $\geq 2$  transition metal compds. chosen from Co, Ce, Ti, Fe, and Cu compds. Cyclohexane was oxidized by O-containing gas in MeCN in the presence of N-hydroxyphthalimide, 0.000093 mol Co(II) octylate, and 0.000099 mol Ti(OPr-i)<sub>4</sub> at 100° under 0.9 MPa for 2.6 h to give cyclohexanone, cyclohexanol, cyclohexyl hydroperoxide, and adipic acid with 47, 8, 25, and 9% selectivity, resp. Remaining of N-hydroxyphthalimide was 73%.

IT **142-71-2**, Copper(II) acetate **516-03-0**, Iron(II) oxalate **1588-79-0** **21679-46-9**, Cobalt(III) acetylacetonate  
 RL: **CAT (Catalyst use); USES (Uses)**  
 (decomposition inhibitor; oxidation of organic compds. without decompns. of imides)  
 RN 142-71-2 CAPLUS  
 CN Acetic acid, copper(2+) salt (8CI, 9CI) (CA INDEX NAME)

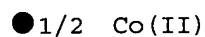
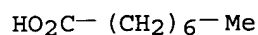


● 1/2 Cu(II)

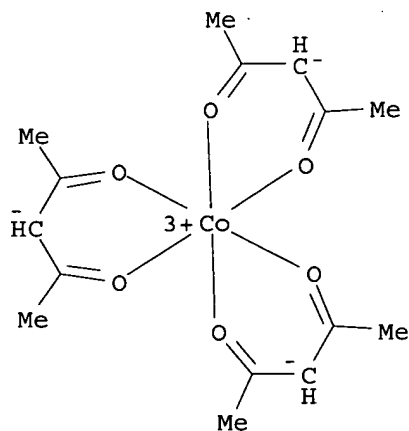
RN 516-03-0 CAPLUS  
 CN Iron, [ethanedioato(2-)- $\kappa$ O1, $\kappa$ O2]- (9CI) (CA INDEX NAME)



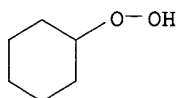
RN 1588-79-0 CAPLUS  
 CN Octanoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



RN 21679-46-9 CAPLUS  
 CN Cobalt, tris(2,4-pentanedionato- $\kappa$ O, $\kappa$ O')-, (OC-6-11)- (9CI)  
 (CA INDEX NAME)



IT 766-07-4P, Cyclohexyl hydroperoxide  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (oxidation of organic compds. without decompns. of imides)  
 RN 766-07-4 CAPLUS  
 CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



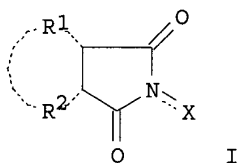
IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidation of organic compds. without decompns. of imides)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 47 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:235931 CAPLUS  
 DOCUMENT NUMBER: 136:294727  
 TITLE: Method for preparing organic compounds using imides  
 and nitric acids  
 INVENTOR(S): Ishii, Yasutaka; Tatsumi, Atsuo; Nakano, Tatsuya  
 PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002088077	A2	20020327	JP 2001-111912	20010410
PRIORITY APPLN. INFO.:			JP 2000-209205	A 20000711
OTHER SOURCE(S):			CASREACT 136:294727; MARPAT 136:294727	

GI



AB Disclosed is a highly selective method with high recovery rate for producing organic compds. by addition reaction and/or substitution reaction under gentle conditions. The addition and/or substitution reaction products are prepared by reacting radical forming compound with radical capturing compound in the presence of imide (I; R1 = alkyl; R2 = aryl, or R1/R2 = aromatic or non-aromatic ring, and X = O or OH) and nitric acid or nitrous acid salt.



IT 7782-44-7, Oxygen, reactions

RL: RGT (Reagent); RACT (Reactant or reagent)

(gas containing; preparation of organic compds. by reacting radical-forming agent

with radical-capturing agent in the presence of imide and nitric or nitrous acid)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



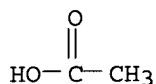
IT 71-48-7, Cobalt acetate 13476-99-8

RL: CAT (Catalyst use); USES (Uses)

(preparation of organic compds. by reacting radical-forming agent with radical-capturing agent in the presence of imide and nitric or nitrous acid)

RN 71-48-7 CAPLUS

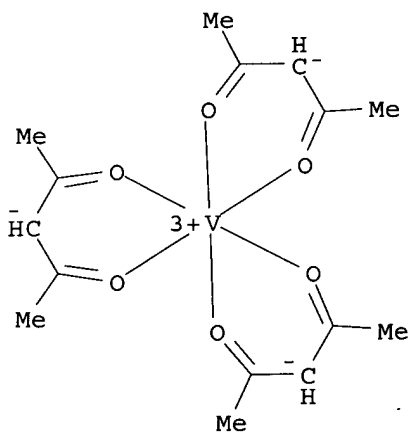
CN Acetic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

RN 13476-99-8 CAPLUS

CN Vanadium, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI)  
(CA INDEX NAME)



IT 766-07-4P, Cyclohexyl hydroperoxide

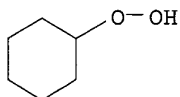
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of organic compds. by reacting radical-forming agent with

radical-capturing agent in the presence of imide and nitric or nitrous acid)

RN 766-07-4 CAPLUS

CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



L34 ANSWER 48 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:405758 CAPLUS

DOCUMENT NUMBER: 136:401466

TITLE: Oxidative process and catalyst system for preparing cyclohexanone, cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas

INVENTOR(S): Murata, Shuzo; Tani, Nobuhiro

PATENT ASSIGNEE(S): Sumitomo Chemical Company Limited, Japan; Daicel Chemical Industries, Ltd.

SOURCE: Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1209143	A1	20020529	EP 2001-127410	20011123
EP 1209143	B1	20040218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2002161056	A2	20020604	JP 2000-357363	20001124
US 2002065436	A1	20020530	US 2001-992012	20011126
US 6459002	B2	20021001		

PRIORITY APPLN. INFO.: JP 2000-357363 A 20001124

OTHER SOURCE(S): CASREACT 136:401466

AB Cyclohexanone, cyclohexanol and/or cyclohexyl hydroperoxide are prepared at a high productivity by the oxidation of cyclohexane with an oxygen-containing gas

using a catalyst system comprising a cyclic N-hydroxyimide (e.g., N-hydroxyphthalimide) and a transition metal compound (e.g., cobalt octoate) in the presence of cyclohexanone, and optional cyclohexanol, which is/are added to the reaction system while conducting the oxidation

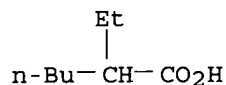
IT 136-52-7, Cobalt octoate

RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidative **catalyst** system for preparing cyclohexanone and cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas)

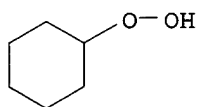
RN 136-52-7 CAPLUS

CN Hexanoic acid, 2-ethyl-, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



● 1/2 Co(II)

IT 766-07-4P, Cyclohexyl hydroperoxide  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (oxidative process and catalyst system for preparing cyclohexanone and cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas)  
 RN 766-07-4 CAPLUS  
 CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidative process and catalyst system for preparing cyclohexanone and cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 49 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2002:386166 CAPLUS  
 DOCUMENT NUMBER: 137:201007  
 TITLE: "Dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions  
 AUTHOR(S): Nardello, Veronique; Herve, Melanie; Alsters, Paul L.; Aubry, Jean-Marie  
 CORPORATE SOURCE: LCOM, Equipe de Recherches "Oxydation et Formulation", ESA CNRS 8009, ENSCL, Villeneuve d'Ascq, 59652, Fr.  
 SOURCE: Advanced Synthesis & Catalysis (2002), 344(2), 184-191  
 CODEN: ASCAF7; ISSN: 1615-4150  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:201007  
 AB The molybdate-catalyzed "dark" singlet oxygenation of hydrophobic compds.

with hydrogen peroxide proceeds efficiently with low catalyst loadings (10-3 mol%) in chlorine-free w/o microemulsions. These micro-heterogeneous systems are composed of sodium dodecyl sulfate (SDS)/n-butanol/water/organic phase, the latter being either a "green" solvent such as Et acetate or a liquid substrate, such as  $\alpha$ -terpinene or  $\beta$ -citronellol. Very high reactor yields with improved product/SDS ratio can be obtained for the "dark" singlet oxygenation of such liquid substrates.

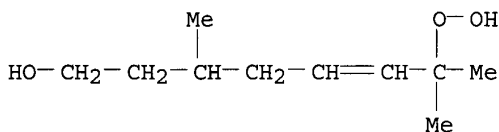
IT 81113-73-7P 81113-74-8P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

("dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions)

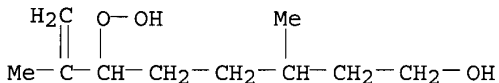
RN 81113-73-7 CAPLUS

CN 5-Octen-1-ol, 7-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 81113-74-8 CAPLUS

CN 7-Octen-1-ol, 6-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



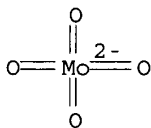
IT 7631-95-0, Sodium molybdate (Na<sub>2</sub>MoO<sub>4</sub>)

RL: CAT (Catalyst use); USES (Uses)

(disproportionation catalyst; "dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions)

RN 7631-95-0 CAPLUS

CN Molybdate (MoO<sub>4</sub><sup>2-</sup>), disodium, (T-4)- (9CI) (CA INDEX NAME)



● 2 Na<sup>+</sup>

IT 7782-44-7, Oxygen, reactions

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC

(Process); **RACT (Reactant or reagent)**

(singlet; "dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 50 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:450919 CAPLUS

DOCUMENT NUMBER: 135:33339

TITLE: Process and catalysts for preparing a ketone, an alcohol and a hydroperoxide by the oxidation of a hydrocarbon

INVENTOR(S): Murata, Shuzo; Tani, Nobuhiro; Asano, Hiroyuki

PATENT ASSIGNEE(S): Sumitomo Chemical Company Limited, Japan; Daicel Chemical Industries, Ltd.

SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1108701	A1	20010620	EP 2000-311105	20001213
EP 1108701	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001233809	A2	20010828	JP 2000-343302	20001110
ES 2197852	T3	20040116	ES 2000-311105	20001213
CN 1302788	A	20010711	CN 2000-137320	20001214
US 2001016670	A1	20010823	US 2000-735926	20001214
US 6479705	B2	20021112		

PRIORITY APPLN. INFO.: JP 1999-354216 A 19991214

OTHER SOURCE(S): CASREACT 135:33339

AB A process for preparing a ketone (e.g., cyclohexanone), an alc. (e.g., cyclohexanol), and/or a hydroperoxide (e.g., cyclohexyl hydroperoxide) in high yield and selectivity comprises reacting a hydrocarbon (e.g., cyclohexane) with mol. oxygen in the presence of a cyclic N-hydroxyimide (e.g., N-hydroxyphthalimide) and a transition metal compound catalyst (e.g., cobalt diacetate) system, where the oxygen-containing gas is supplied to the reaction system and at the same time a gas containing 1-10% (by volume) of oxygen is discharged from the reaction system.

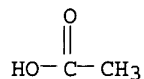
IT 71-48-7, Cobalt diacetate 1588-79-0, Cobalt dioctanoate 14284-89-0, ManganeseIII acetylacetonate

RL: CAT (Catalyst use); USES (Uses)

(catalysts for preparing a ketone and an alc. and a hydroperoxide by the oxidation of a hydrocarbon)

RN 71-48-7 CAPLUS

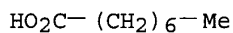
CN Acetic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

RN 1588-79-0 CAPLUS

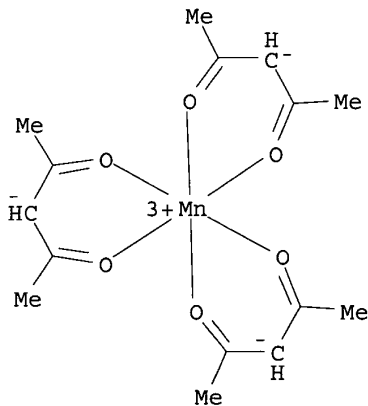
CN Octanoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

RN 14284-89-0 CAPLUS

CN Manganese, tris(2,4-pentanedionato- $\kappa\text{O},\kappa\text{O}'$ )-, (OC-6-11)- (9CI)  
(CA INDEX NAME)



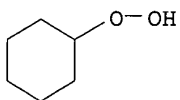
IT 766-07-4P, Cyclohexyl hydroperoxide

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process and catalysts for preparing a ketone and an alc. and a hydroperoxide by the oxidation of a hydrocarbon)

RN 766-07-4 CAPLUS

CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(process and catalysts for preparing a ketone and an alc. and a  
hydroperoxide by the oxidation of a hydrocarbon)  
RN 7782-44-7 CAPLUS  
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 51 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:883290 CAPLUS

DOCUMENT NUMBER: 136:216383

TITLE: Dioxygen affinity and catalytic performance of  
bis-(furaldehyde) Schiff bases Co(II) complexes in  
cyclohexene oxidation

AUTHOR(S): Sun, Bin; Chen, Jun Ru; Hu, Jia Yuan; Li, Xian Jun

CORPORATE SOURCE: Department of Chemistry, Sichuan University, Chengdu,  
610064, Peop. Rep. China

SOURCE: Chinese Chemical Letters (2001), 12(11), 1043-1046  
CODEN: CCLEE7; ISSN: 1001-8417

PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:216383

AB Oxygenation consts. and thermodyn. parameters  $\Delta H^\circ$  and  
 $\Delta S^\circ$  of Co (II) complexes with three bis(furaldehyde) Schiff  
bases (1, 2, 3, 4) were obtained by measuring saturated dioxygen uptake of  
these complexes in pyridine at different temperature. These complexes could  
activate mol. O and were used as catalysts in cyclohexene oxidation. The  
influence of ligand structure on the dioxygen affinity and catalytic  
activity of the complexes were discussed.

IT 7782-44-7, Oxygen, reactions  
RL: CPS (Chemical process); PEP (Physical, engineering or chemical  
process); PRP (Properties); RCT (Reactant); PROC (Process);  
RACT (Reactant or reagent)  
(carrier mimic for; dioxygen affinity and catalytic performance of  
bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7646-79-9, Cobaltous chloride, reactions  
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or  
reagent); USES (Uses)  
(catalyst precursor; dioxygen affinity and catalytic  
performance of bis(furaldehyde) Schiff base Co(II) complexes in  
cyclohexene oxidation)  
RN 7646-79-9 CAPLUS

CN Cobalt chloride (CoCl<sub>2</sub>) (8CI, 9CI) (CA INDEX NAME)

Cl-Co-Cl

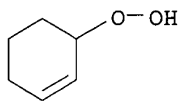
IT 4845-05-0P

RL: **BYP (Byproduct); PREP (Preparation)**

(dioxygen affinity and catalytic performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)

RN 4845-05-0 CAPLUS

CN Hydroperoxide, 2-cyclohexen-1-yl (9CI) (CA INDEX NAME)



IT 402594-30-3 402594-31-4 402594-32-5

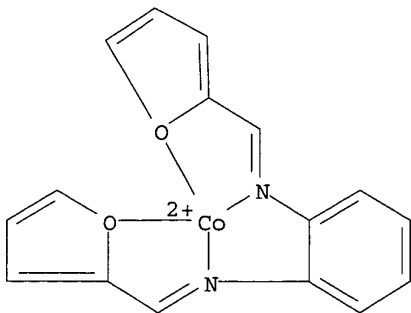
402594-33-6

RL: **CAT (Catalyst use); CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)**

(dioxygen affinity and **catalytic** performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)

RN 402594-30-3 CAPLUS

CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-benzenediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)

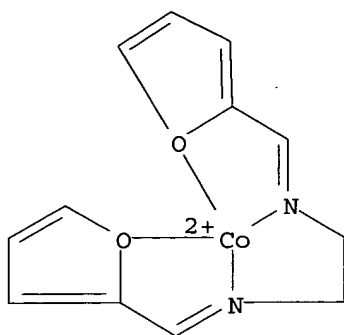


●<sub>2</sub> Cl<sup>-</sup>

RN 402594-31-4 CAPLUS

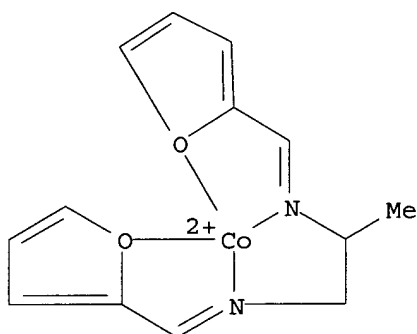
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-ethanediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)





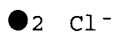
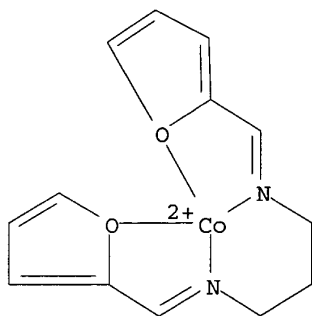
● 2 Cl<sup>-</sup>

RN 402594-32-5 CAPLUS  
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-propanediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)



● 2 Cl<sup>-</sup>

RN 402594-33-6 CAPLUS  
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,3-propanediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)



IT 402594-38-1 402594-39-2 402594-40-5

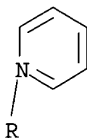
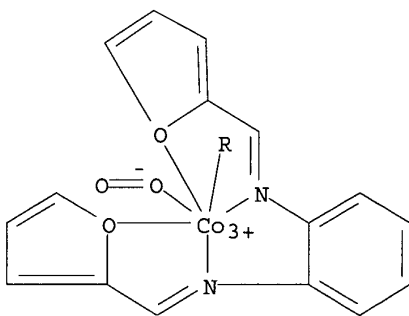
402594-41-6

RL: CAT (Catalyst use); CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(oxygen carrier; dioxygen affinity and **catalytic** performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)

RN 402594-38-1 CAPLUS

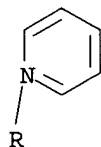
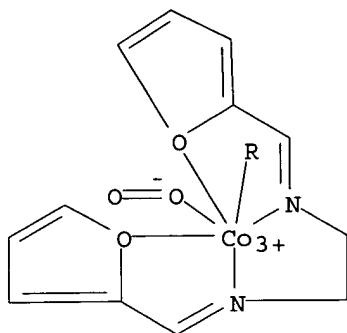
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-benzenediamine-κN,κN'] (pyridine) superoxido-, (OC-6-43)- (9CI) (CA INDEX NAME)



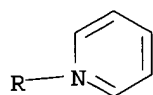
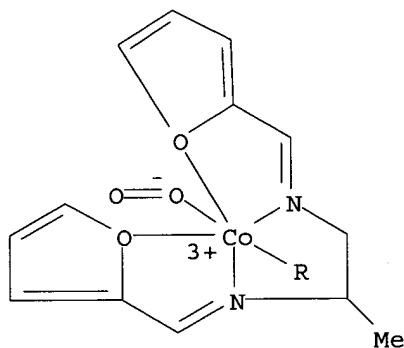
RN 402594-39-2 CAPLUS

CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-ethanediamine-

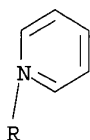
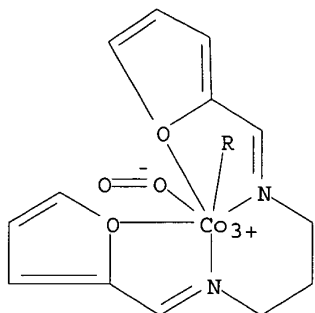
$\kappa N, \kappa N'$ ] (pyridine)superoxido-, (OC-6-43)- (9CI) (CA INDEX  
NAME)



RN 402594-40-5 CAPLUS  
CN Cobalt (2+), [N,N'-bis[(2-furanyl- $\kappa O$ )methylene]-1,2-propanediamine- $\kappa N, \kappa N'$ ] (pyridine)superoxido-, (OC-6-65)- (9CI) (CA INDEX  
NAME)



RN 402594-41-6 CAPLUS  
CN Cobalt (2+), [N,N'-bis[(2-furanyl- $\kappa O$ )methylene]-1,3-propanediamine- $\kappa N, \kappa N'$ ] (pyridine)superoxido-, (OC-6-43)- (9CI) (CA INDEX  
NAME)

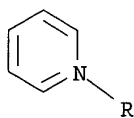
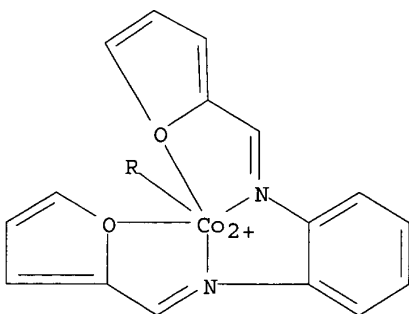


IT 402594-34-7 402594-35-8 402594-36-9  
402594-37-0

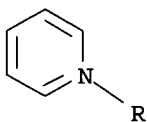
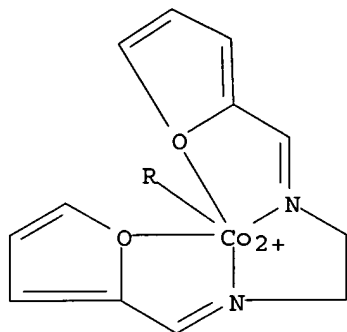
RL: **CAT** (Catalyst use); CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)  
(oxygenation of **precatalyst**; dioxygen affinity and **catalytic** performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)

RN 402594-34-7 CAPLUS

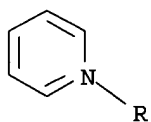
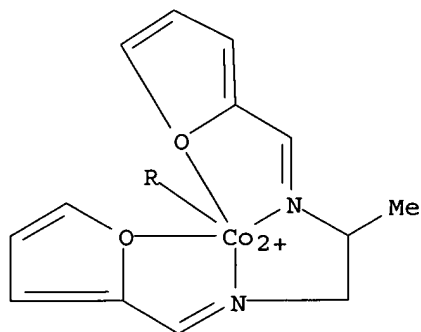
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-benzenediamine-κN,κN'] (pyridine)-, (SP-5-32)- (9CI) (CA INDEX NAME)



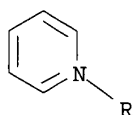
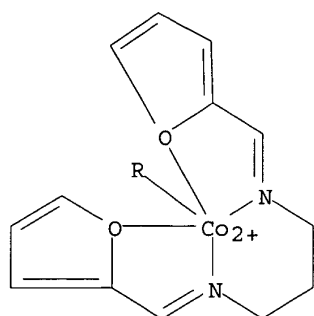
RN 402594-35-8 CAPLUS  
CN Cobalt(2+), [N,N'-bis[(2-furanyl- $\kappa$ O)methylene]-1,2-ethanediamine- $\kappa$ N, $\kappa$ N'] (pyridine)-, (SP-5-32)- (9CI) (CA INDEX NAME)



RN 402594-36-9 CAPLUS  
CN Cobalt(2+), [N,N'-bis[(2-furanyl- $\kappa$ O)methylene]-1,2-propanediamine- $\kappa$ N, $\kappa$ N'] (pyridine)-, (SP-5-54)- (9CI) (CA INDEX NAME)



RN 402594-37-0 CAPLUS  
CN Cobalt(2+), [N,N'-bis[(2-furanyl- $\kappa$ O)methylene]-1,3-propanediamine- $\kappa$ N, $\kappa$ N'] (pyridine)-, (SP-5-32)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 52 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2000:742044 CAPLUS  
 DOCUMENT NUMBER: 133:281926  
 TITLE: Singlet oxygen oxidation of organic substrates  
 INVENTOR(S): Aubry, Jean-Marie; Rataj-Nardello, Veronique; Alsters, Paul  
 PATENT ASSIGNEE(S): DSM Fine Chemicals Austria G.m.b.H., Austria  
 SOURCE: PCT Int. Appl., 18 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000061524	A1	20001019	WO 2000-EP2552	20000323
W: AE, AL, AM, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AT 9900647	A	20010515	AT 1999-647	19990413
AT 408546	B	20011227		
CA 2369589	AA	20001019	CA 2000-2369589	20000323
EP 1169281	A1	20020109	EP 2000-922539	20000323
EP 1169281	B1	20040218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002541227	T2	20021203	JP 2000-610802	20000323
AT 259764	E	20040315	AT 2000-922539	20000323

PT 1169281	T	20040531	PT 2000-922539	20000323
ES 2211533	T3	20040716	ES 2000-922539	20000323
PRIORITY APPLN. INFO.:			AT 1999-647	A 19990413
			WO 2000-EP2552	W 20000323

OTHER SOURCE(S): CASREACT 133:281926

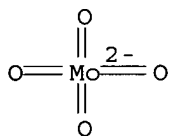
AB The invention relates to a method for oxidizing organic substrates using 1O<sub>2</sub> in which hydrophobic organic substrates that react with 1O<sub>2</sub> are added to an organic solvent in the presence of a heterogeneous or homogeneous catalyst with 30-70% being comprised of H<sub>2</sub>O<sub>2</sub>. Afterwards, H<sub>2</sub>O<sub>2</sub> is catalytically decomposed into water and 1O<sub>2</sub>, and the oxidation into corresponding oxidation products ensues. Thus, α-terpinene is added to methanol containing Na<sub>2</sub>MoO<sub>4</sub>·2H<sub>2</sub>O followed by 45 μl H<sub>2</sub>O<sub>2</sub> to give 100% ascaridol.

IT 7631-95-0, Sodium molybdate

RL: CAT (Catalyst use); USES (Uses)

(oxidation of organic substrates with singlet oxygen in the presence of a heterogeneous or homogeneous catalyst)

RN 7631-95-0 CAPLUS

CN Molybdate (MoO<sub>4</sub><sup>2-</sup>), disodium, (T-4)- (9CI) (CA INDEX NAME)● 2 Na<sup>+</sup>

IT 7782-44-7D, Oxygen, singlet, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation of organic substrates with singlet oxygen in the presence of a heterogeneous or homogeneous catalyst)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



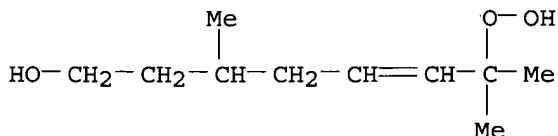
IT 81113-73-7P 81113-74-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

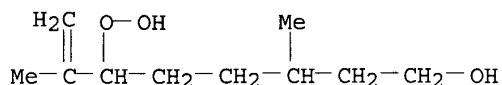
(oxidation of organic substrates with singlet oxygen in the presence of a heterogeneous or homogeneous catalyst)

RN 81113-73-7 CAPLUS

CN 5-Octen-1-ol, 7-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 81113-74-8 CAPLUS  
 CN 7-Octen-1-ol, 6-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 53 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:12136 CAPLUS

DOCUMENT NUMBER: 142:56002

TITLE: An improved process for the preparation of phenylpropylcarbinyl esters of organic acids

INVENTOR(S): Shende, Bansidhar Wasudeo; Shah, Naresh Fulchand; Chaudhuri, Basab

PATENT ASSIGNEE(S): Herdillia Chemicals Ltd., India

SOURCE: Indian, 16 pp.

CODEN: INXXAP

DOCUMENT TYPE: Patent

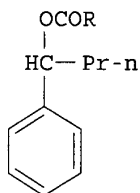
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 185059	A	20001028	IN 1996-BO103	19960222
PRIORITY APPLN. INFO.:			IN 1996-BO103	19960222
OTHER SOURCE(S):		CASREACT 142:56002; MARPAT 142:56002		

GI



AB An improved process for the preparation of phenylpropylcarbinyl esters of the formula I wherein R represents an alkyl group is reported. The process involved oxidation of n-butylbenzene with oxygen or a gas containing it, at a temperature in the range of 120 to 140°C, pH in the range of 5.5 to 6.5, maintaining the content of water in the reaction mixture in the range of 2 to 8% weight/weight, pressure in the range of 2 to 10 kg/cm<sup>2</sup> and the space velocity of the oxygen-containing gas in the range of 1 to 4 cm/s, gave a mixture containing unreacted n-butylbenzene, 1-phenylbutyl hydroperoxide 1-phenyl-1-butanone and phenylpropylcarbinol. Further, conversion of 1-phenylbutyl hydroperoxide from the above mixture to phenylpropylcarbinol by direct hydrogenation with hydrogen at a temperature in the range of 30 to



70°C and pressure in the range of 3 to 10 kg/cm<sup>2</sup> in the presence of a hydrogenation catalyst gave a mixture containing n-butylbenzene and 1-phenyl-1-butanone. The reduction of 1-phenyl-1-butanone in the mixture obtained from the previous step by hydrogenation at a temperature in the range of 80 to 180°C and a pressure in the range of 5-75 kg/cm<sup>2</sup> in the presence of a hydrogenation catalyst resulted in a new mixture containing n-butylbenzene and phenylpropylcarbinol. Finally, phenylpropylcarbinol was separated from the mixture by fractional distillation, which upon acylation yielded the title compds.

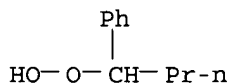
IT 7440-02-0, Raney nickel, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst hydrogenation; industrial preparation of phenylpropylcarbiny l esters from phenylpropylcarbinol via oxidation of butylbenzene followed by hydrogenation of phenylbutyl hydroperoxide and phenylbutanone intermediates)  
 RN 7440-02-0 CAPLUS  
 CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (industrial preparation of phenylpropylcarbiny l esters from phenylpropylcarbinol via oxidation of butylbenzene followed by hydrogenation of phenylbutyl hydroperoxide and phenylbutanone intermediates)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

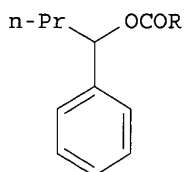
IT 58687-89-1P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; industrial preparation of phenylpropylcarbiny l esters from phenylpropylcarbinol via oxidation of butylbenzene followed by hydrogenation of phenylbutyl hydroperoxide and phenylbutanone intermediates)  
 RN 58687-89-1 CAPLUS  
 CN Hydroperoxide, 1-phenylbutyl (9CI) (CA INDEX NAME)



L34 ANSWER 54 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2005:55319 CAPLUS  
 DOCUMENT NUMBER: 142:93537

TITLE: An improved process for the preparation of  
phenylpropylcarbinyl esters of organic acids  
INVENTOR(S): Shende, Bansidhar Wasudeo; Shah, Naresh Fulchand;  
Chaudhuri, Basab  
PATENT ASSIGNEE(S): Herdillia Chemicals Ltd., India  
SOURCE: Indian, 14 pp.  
CODEN: INXXAP  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 185058	A	20001028	IN 1996-BO102	19960222
PRIORITY APPLN. INFO.:			IN 1996-BO102	19960222
OTHER SOURCE(S):	CASREACT 142:93537; MARPAT 142:93537			
GI				



AB An improved process for the preparation of phenylpropylcarbinyl esters I (R = alkyl group) from n-butylbenzene which comprises, oxidation of n-butylbenzene by oxygen of a gas containing it under specified condition resulted in a mixture

containing unreacted n-butylbenzene, 1-phenylbutyl hydroperoxide, 1-phenyl-1-butanone and phenylpropylcarbinol. Addition of cyclic olefin to above mixture obtained from previous step at a temperature in the range of 60 to

110°C under autogenous pressure in the presence of an epoxidn. catalyst resulted in conversion of 1-phenylbutyl hydroperoxide present in the mixture to phenylpropylcarbinol and the cyclic olefin to its epoxide, separating the unconverted cyclic olefin and its epoxide by fractional distillation

was done to obtain the appropriate epoxide as a co-product. Reduction of 1-phenyl-1-butanone in the mixture obtained from the above step via hydrogenation at a temperature in the range of 80 to 180°C and a pressure in the range of 5-75 kg/cm<sup>2</sup> in the presence of a hydrogenation catalyst yielded a mixture containing n-butylbenzene and phenylpropylcarbinol.

Separation of phenylpropylcarbinol from the mixture was achieved by fractional distillation. Finally, acylation of phenylpropylcarbinol by conventional methods afforded the phenylpropylcarbinyl esters I.

IT 7440-02-0, Raney nickel, uses

RL: CAT (Catalyst use); USES (Uses)

(catalysts hydrogenation; industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by epoxidn. of cyclohexene by phenylbutyl hydroperoxide intermediate and subsequent hydrogenation)

RN 7440-02-0 CAPLUS  
 CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

IT 30568-96-8, Molybdenum stearate  
 RL: CAT (Catalyst use); USES (Uses)  
 (epoxidn. catalyst; industrial preparation of phenylpropylcarbiny  
 esters from phenylpropylcarbinol via oxidation of butylbenzene followed by  
 epoxidn. of cyclohexene by phenylbutyl hydroperoxide intermediate and  
 subsequent hydrogenation)  
 RN 30568-96-8 CAPLUS  
 CN Octadecanoic acid, molybdenum salt (9CI) (CA INDEX NAME)

$\text{HO}_2\text{C}-(\text{CH}_2)_{16}-\text{Me}$

●x Mo(x)

IT 58687-89-1P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN  
 (Synthetic preparation); PREP (Preparation); RACT (Reactant  
 or reagent)  
 (industrial preparation of phenylpropylcarbiny esters from  
 phenylpropylcarbinol via oxidation of butylbenzene followed by epoxidn. of  
 cyclohexene by phenylbutyl hydroperoxide intermediate and subsequent  
 hydrogenation)  
 RN 58687-89-1 CAPLUS  
 CN Hydroperoxide, 1-phenylbutyl (9CI) (CA INDEX NAME)

Ph  
 |  
 $\text{HO}-\text{O}-\text{CH}-\text{Pr}-\text{n}$

IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidizing agent; industrial preparation of phenylpropylcarbiny esters from  
 phenylpropylcarbinol via oxidation of butylbenzene followed by epoxidn. of  
 cyclohexene by phenylbutyl hydroperoxide intermediate and subsequent  
 hydrogenation)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

$\text{O}=\text{O}$

L34 ANSWER 55 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:426679 CAPLUS

DOCUMENT NUMBER: 133:266543

TITLE: The oxidation of ethylbenzene and other alkylaromatics by dioxygen catalyzed by iron(III) tetrakis(pentafluorophenyl)porphyrin and related iron porphyrins

AUTHOR(S): Evans, Steven; Lindsay Smith, John R.

CORPORATE SOURCE: Department of Chemistry, University of York, York, YO10 5DD, UK

SOURCE: Perkin 2 (2000), (7), 1541-1552

CODEN: PRKTFO

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:266543

AB The oxidation of ethylbenzene with dioxygen catalyzed by iron(III) porphyrins in a solvent free system was studied over the temperature range 30-110 °C. The time dependence of the formation of the three main products, 1-phenylethanol, acetophenone and 1-phenylethyl hydroperoxide, and the fate of the iron porphyrin are interpreted in terms of a free radical autoxidn. mechanism. The yields of the oxidation products are determined

by the rate of reaction and by the lifetime of the catalyst. Catalyst degradation is shown to involve reaction of the porphyrin ligand with 1-phenylethoxyl and 1-phenylethylperoxyl radicals. The disadvantages of increased induction periods and longer reaction times of the oxidns. observed at lower reaction temps. are counter balanced by increased catalyst turnovers. Less extensive studies on the oxidns. of toluene, cumene, (2-methylpropyl)benzene and tert-butylbenzene support the overall mechanism proposed for ethylbenzene. A comparative study using the catalysts iron(III) 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)porphyrin and iron(III) tetrakis(pentafluorophenyl)porphyrin and five of its derivs. reveals that halogenation of the  $\beta$ -pyrrole positions markedly increases the activity of the catalysts but not the stability of the porphyrin towards degradation. The highest yields were obtained with the  $\mu$ -oxo dimer of iron(III) tetrakis(pentafluorophenyl)porphyrin and iron(III) tetrakis(4-dimethylamino-2,3,5,6-tetrafluorophenyl)porphyrin.

IT 81245-20-7,  $\mu$ -Oxobis[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato]diiron 107053-17-8,

Chloro[octabromotetrakis(2,6-dichlorophenyl)porphyrinato]iron

RL: CAT (Catalyst use); USES (Uses)

(oxidation of (alkyl)benzenes by dioxygen catalyzed by iron porphyrins)

RN 81245-20-7 CAPLUS

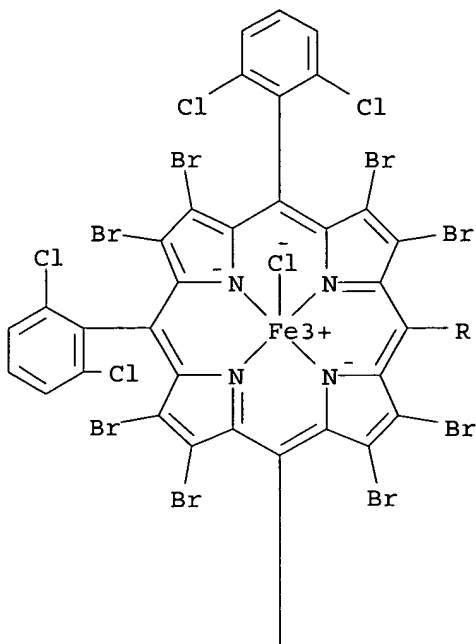
CN Iron,  $\mu$ -oxobis[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)- $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]di- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

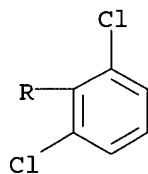
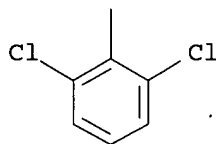
RN 107053-17-8 CAPLUS

CN Iron, chloro[2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)- $\kappa$ N21, $\kappa$ N22, $\kappa$ N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

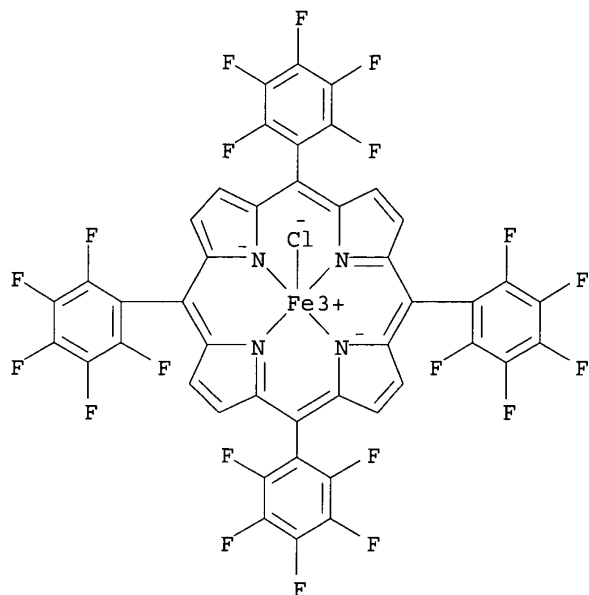
PAGE 1-A



PAGE 2-A

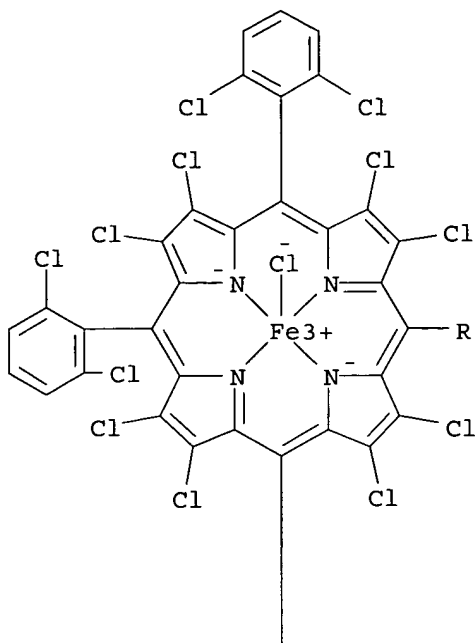


IT **36965-71-6P**, Chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinatoiron(III)]  
 RL: **CAT (Catalyst use)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (oxidation of (alkyl)benzenes by dioxygen **catalyzed** by iron porphyrins)  
 RN 36965-71-6 CAPLUS  
 CN Iron, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)-(9CI) (CA INDEX NAME)

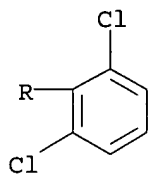
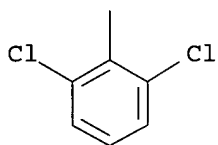


IT 120676-09-7P, Chloro[octachlorotetrakis(2,6-dichlorophenyl)porphyrinato]iron 131917-66-3P  
 134131-11-6P, Iron(III) 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin 177532-06-8P,  
 Chloro[5,10,15,20-tetrakis(tetrafluoro4-phenoxyphenyl)-21H,23H-porphinatoiron(III)  
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
 (oxidation of (alkyl)benzenes by dioxygen catalyzed by iron porphyrins)  
 RN 120676-09-7 CAPLUS  
 CN Iron, chloro[2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

PAGE 1-A

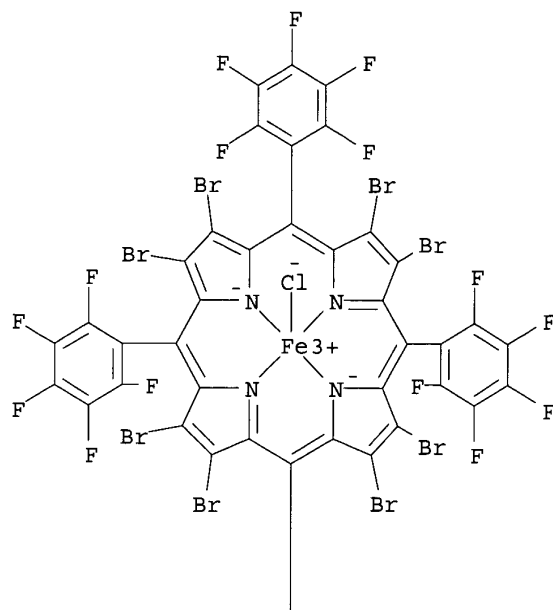


PAGE 2-A

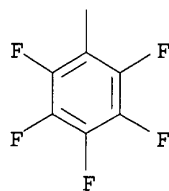


RN 131917-66-3 CAPLUS  
 CN Iron, chloro[2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5÷12)- (9Cl) (CA INDEX NAME)

PAGE 1-A



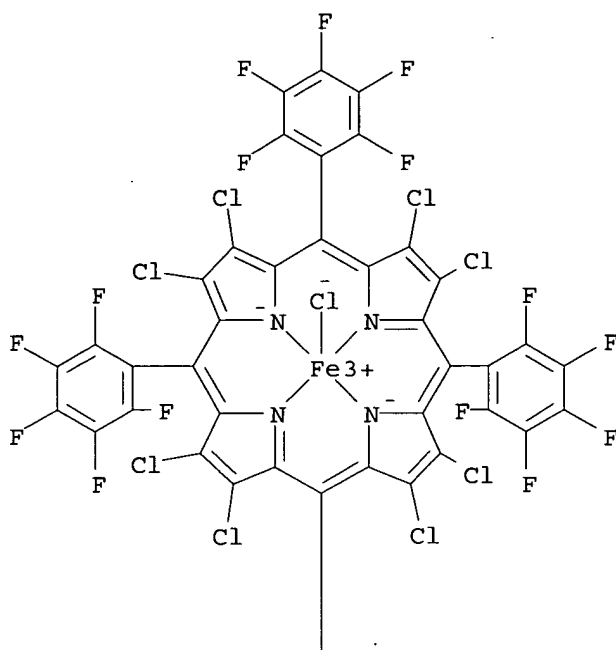
PAGE 2-A



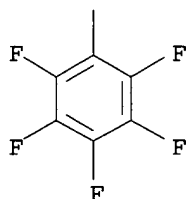
RN 134131-11-6 CAPLUS  
 CN Iron, chloro[2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



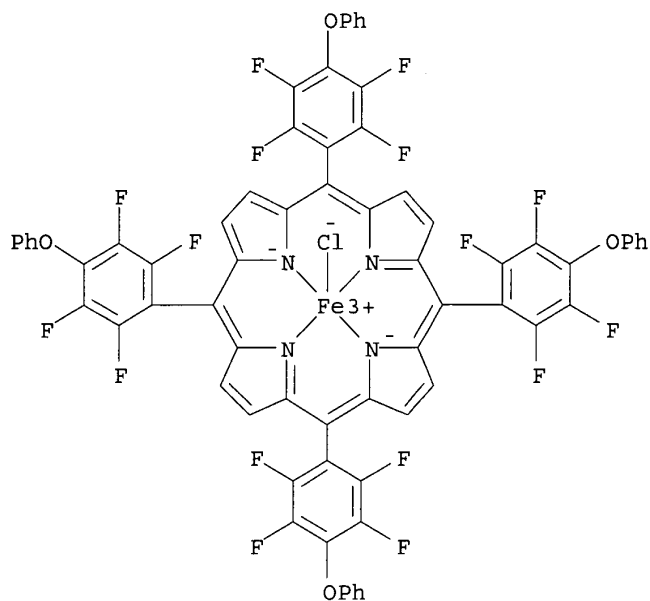
PAGE 1-A



PAGE 2-A



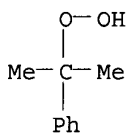
RN 177532-06-8 CAPLUS  
 CN Iron, chloro[5,10,15,20-tetrakis(2,3,5,6-tetrafluoro-4-phenoxyphenyl)-  
 21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-,  
 (SP-5-12)-(9CI) (CA INDEX NAME)



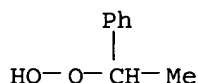
IT 7782-44-7, Dioxygen, reactions  
 RL: **RCT (Reactant); RACT (Reactant or reagent)**  
 (oxidation of (alkyl)benzenes by dioxygen catalyzed by iron porphyrins)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 80-15-9P, Cumene hydroperoxide  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (oxidation of cumene by dioxygen catalyzed by iron porphyrins)  
 RN 80-15-9 CAPLUS  
 CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



IT 3071-32-7P, 1-Phenylethyl hydroperoxide  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (oxidation of ethylbenzene by dioxygen catalyzed by iron porphyrins)  
 RN 3071-32-7 CAPLUS  
 CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 56 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:296195 CAPLUS

DOCUMENT NUMBER: 133:43120

TITLE: Ozonation of 1,1,2,2-tetraphenylethene revisited: evidence for electron-transfer oxygenations

AUTHOR(S): Schank, Kurt; Beck, Horst; Buschlinger, Michael; Eder, Jorg; Heisel, Thomas; Pistorius, Susanne; Wagner, Christiane

CORPORATE SOURCE: Department of Organic Chemistry, University of Saarland, Saarbrücken, D-66041, Germany

SOURCE: Helvetica Chimica Acta (2000), 83(4), 801-826

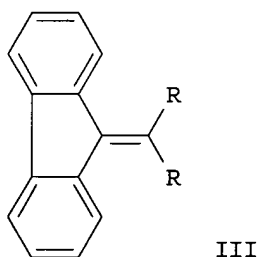
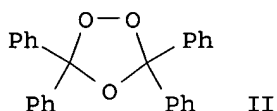
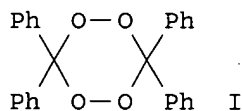
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

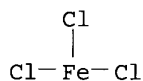
GI



AB Ozonolysis of 1,1,2,2-tetraphenylethene (TPE, 1) were described many times in the literature, but the reports are contradictory. This reaction is particularly important for understanding the mechanism of alkene ozonolysis, in view of possible stabilization of reactive intermediates by aryl groups. Thus, systematic studies of ozonolysis in both aprotic solvents and in protic solvents are reported here. Attention is directed to the following details that were underestimated in the past: (i) the actual electronic structure of ground-state ozone (O<sub>3</sub>), (ii) differentiation between strained and unstrained alkenes, (iii) the significance of both the O<sub>3</sub> concentration and the TPE concentration, (iv) the influence of various solvents, including pyridine, (v) the influence of the reaction temperature, (vi) the role of electron-transfer catalysis (ETC) and, (vii) the effect of structural modifications. Results suggest that ozonolysis of TPE (1) does not include a 1,3-dipolar reaction step, but represents a particularly interesting example of electron-donor (TPE)/electron-acceptor (O<sub>3</sub>) redox chemical. The present studies include several crucial results.

First, pure 3,3,6,6-tetraphenyltetroxane (I, m.p. 221° (dec.)) and pure tetraphenylethylene ozonide (II, m.p. 153° (dec.)) are prepared for the 1st time, although I and II have long been known. Second, the singlet diradical character of O<sub>3</sub>, lessened by hypervalent-electron interaction and predicted by different calcns., is evidenced via reaction with the spin trap galvinoxyl [2,6-bis(1,1-dimethylethyl)-4-{[3,5-bis(1,1-dimethylethyl)-4-oxocyclohexa-2,5-dien-1-ylidene]methyl}phenoxy] (8), and the zwitterionic reaction behavior of ground-state O<sub>3</sub> is ruled out. Third, the electron-acceptor ability of O<sub>3</sub> is evidenced by reactions with suitable tetraaryl ethylenes: it is enhanced by addition of catalytic amts. of protons or Lewis acids. Fourth, the observed distribution of the O<sub>3</sub> O-atoms to the 2 different olefinic C-atoms of the unsym. alkene III (R = p-MeOC<sub>6</sub>H<sub>4</sub>) is in full agreement with an initial single-electron transfer (SET) step, followed by a radical mono-oxygenation to cause the crucial C,C cleavage. Final dioxygenation should lead to the generally (ozonides, tetroxanes, hydroperoxides). The regioselectivity is inconsistent with the expected decay of an intermediate primary ozonide. Finally, the treatment of 1,2-bis(4-methoxyphenyl)acenaphthylene (36) with O<sub>3</sub> (simultaneous transfer of 3 O-atoms) leads to the same exptl. result as a stepwise transfer of one O-atom followed by a transfer of 2 O-atoms.

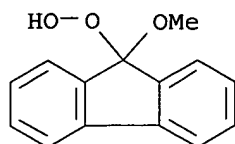
IT 7705-08-0, Ferric chloride, uses  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (electron transfer **catalyst**; electron-transfer oxygenations  
 in ozonation of 1,1,2,2-tetraphenylethene)  
 RN 7705-08-0 CAPLUS  
 CN Iron chloride (FeCl<sub>3</sub>) (8CI, 9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions  
 RL: PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**  
 (electron-transfer oxygenations in ozonation of 1,1,2,2-tetraphenylethene)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 275822-22-5P  
 RL: **RCT (Reactant)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**  
 (electron-transfer oxygenations in ozonation of 1,1,2,2-tetraphenylethene)  
 RN 275822-22-5 CAPLUS  
 CN Hydroperoxide, 9-methoxy-9H-fluoren-9-yl (9CI) (CA INDEX NAME)



IT 7440-50-8, Copper, uses  
 RL: CAT (Catalyst use); USES (Uses)  
 (reductive coupling catalyst; electron-transfer oxygenations  
 in ozonation of 1,1,2,2-tetraphenylethene)  
 RN 7440-50-8 CAPLUS  
 CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

REFERENCE COUNT: 155 THERE ARE 155 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L34 ANSWER 57 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:135769 CAPLUS

DOCUMENT NUMBER: 132:250818

TITLE: Catalytic oxidation of a trialkyl-substituted phenol  
 and aniline with biomimetic Schiff base complexes

AUTHOR(S): Knaudt, Jutta; Forster, Stefan; Bartsch, Ulrich;  
 Rieker, Anton; Jager, Ernst-G.

CORPORATE SOURCE: Institute of Inorganic and Analytical Chemistry,  
 University of Jena, Jena, D-07743, Germany

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences  
 (2000), 55(1), 86-93

CODEN: ZNBSEN; ISSN: 0932-0776

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The catalytic oxidation of 2,4,6-tri-tert-butylphenol and  
 2,4,6-tri-tert-butylaniline with mol. oxygen and tert-butylhydroperoxide  
 was investigated using biomimetic Mn-, Fe- and Co-complexes as catalysts.  
 The catalytic activity and product distribution were determined and compared  
 with those observed in the reactions of the well-known Co(salen) complex.

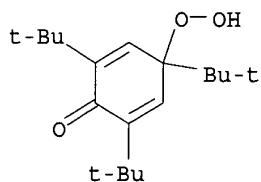
IT 33919-05-0P

RL: BYP (Byproduct); PREP (Preparation)

(byproduct; catalytic oxidation of trialkyl-substituted phenol and aniline  
 with biomimetic Schiff base complexes)

RN 33919-05-0 CAPLUS

CN 2,5-Cyclohexadien-1-one, 2,4,6-tris(1,1-dimethylethyl)-4-hydroperoxy-  
 (9CI) (CA INDEX NAME)



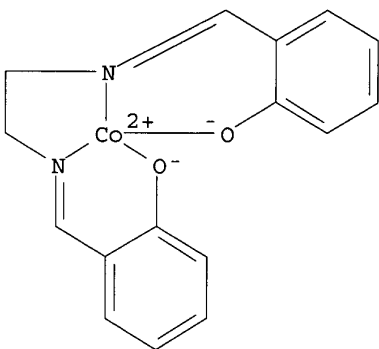
IT 14167-18-1 63510-39-4 63510-43-0  
 63510-45-2 98262-52-3 99392-76-4  
 127899-91-6 182245-44-9

RL: CAT (Catalyst use); USES (Uses)

(catalytic oxidation of trialkyl-substituted phenol and aniline  
 with biomimetic Schiff base complexes)

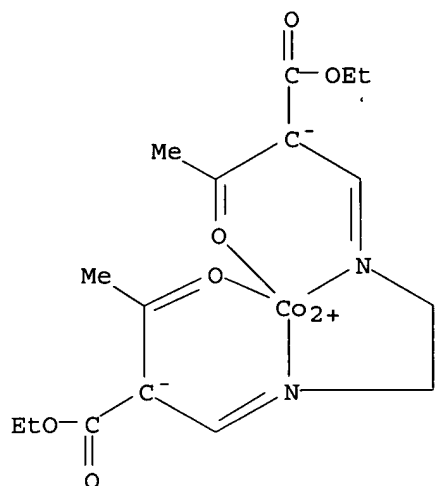
RN 14167-18-1 CAPLUS

CN Cobalt, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[pheno-  
 lato-κO]](2-)]-, (SP-4-2)-(9CI) (CA INDEX NAME)



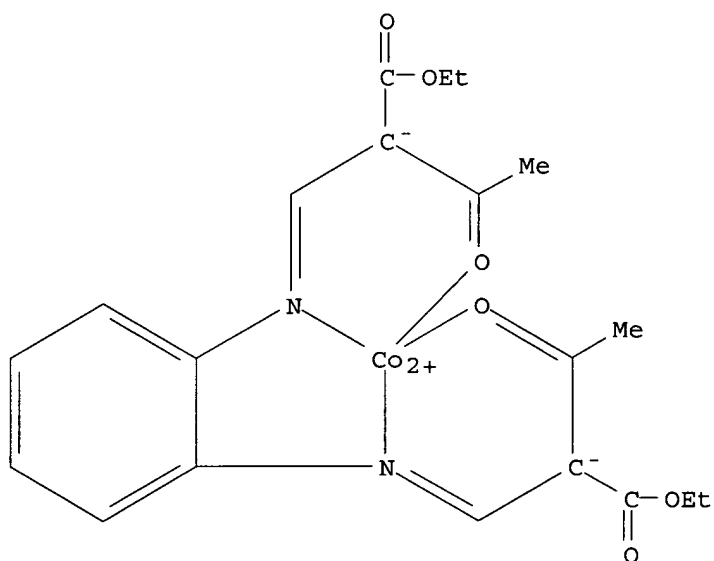
RN 63510-39-4 CAPLUS

CN Cobalt, [[diethyl 2,2'-[1,2-ethanediylbis[(nitrilo-  
 κN)methylidyne]]bis[3-(oxo-κO)butanoato]](2-)]-, (SP-4-2)-  
 (9CI) (CA INDEX NAME)



RN 63510-43-0 CAPLUS

CN Cobalt, [[diethyl 2,2'-[1,2-phenylenebis[(nitrilo-  
κN)methylidyne]]bis[3-(oxo-κO)butanoato]](2-)]-, (SP-4-2)-  
(9CI) (CA INDEX NAME)

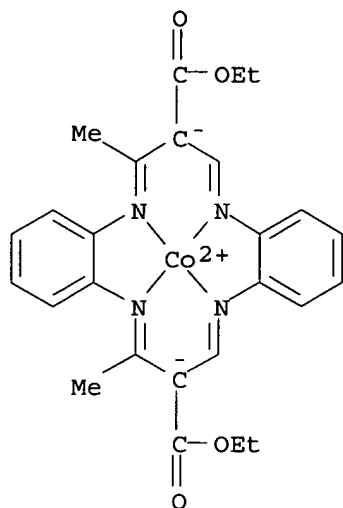


RN 63510-45-2 CAPLUS

CN Cobalt, [[tetraethyl 2,2'-[1,2-phenylenebis[(nitrilo-  
κN)methylidyne]]bis[propanedioato-κO1']](2-)]-, (SP-4-2)-  
(9CI) (CA INDEX NAME)

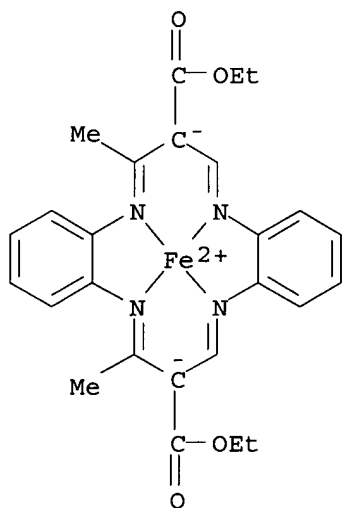






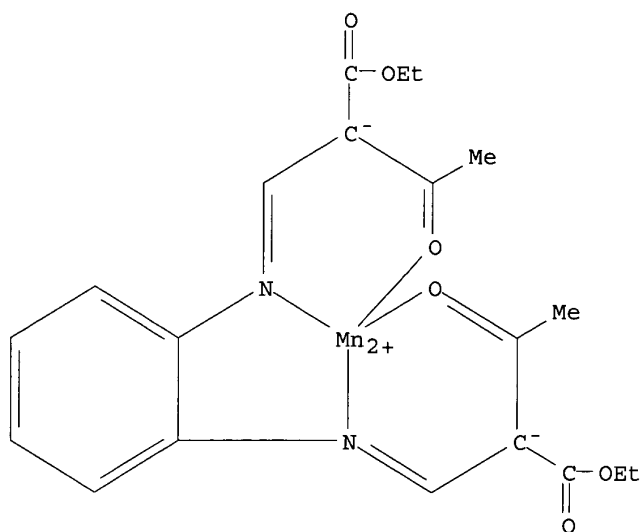
RN 127899-91-6 CAPLUS

CN Iron, [diethyl 7,16-dihydro-6,17-dimethyldibenzo[b,i][1,4,8,11]tetraazacyclotetradecine-7,16-dicarboxylato(2-)-κN5,κN9,κN14,κN18]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 182245-44-9 CAPLUS

CN Manganese, [[diethyl 2,2'-[1,2-phenylenedi(nitrilo-κN)]bis[3-(oxo-κO)butanoato]](2-)]- (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(catalytic oxidation of trialkyl-substituted phenol and aniline with biomimetic Schiff base complexes)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 58 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:430103 CAPLUS

DOCUMENT NUMBER: 129:110412

TITLE: Tertiary butyl alcohol absorption process for recovering propylene and isobutane in oxidation of isobutane and epoxidation of propylene

INVENTOR(S): Chess, David Durham; Pottratz, David George; Nguyen, Eileen Tovan; Culbreth, William Kemp, III

PATENT ASSIGNEE(S): Huntsman Specialty Chemicals Corp., USA

SOURCE: U.S., 7 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5773634	A	19980630	US 1996-749190	19961114
PRIORITY APPLN. INFO.:			US 1996-749190	19961114
AB The liquid and gaseous products formed by reacting oxygen with isobutane in				

an oxidation reactor are sep. processed; the liquid reaction product being charged to a distillation zone and separated into a lower boiling isobutane fraction

and a higher boiling fraction comprising tert-Bu alc. and tert-Bu hydroperoxide; the gaseous reaction product comprising inert gases and vaporized and/or entrained isobutane being cooled by an amount sufficient to condense isobutane contained therein for recycle to the oxidation reactor; the remaining gases, including isobutane being charged to a tert-Bu alc. absorber to obtain a solution of isobutane in tert-Bu alc. that is recycled to the distillation zone.

IT 7439-98-7, Molybdenum, uses  
RL: **CAT (Catalyst use)**; **USES (Uses)**  
(epoxidn. **catalyst**; process for recovering propylene and isobutane by tert-Bu alc. absorption in oxidation of isobutane and epoxidn. of propylene)  
RN 7439-98-7 CAPLUS  
CN Molybdenum (8CI, 9CI) (CA INDEX NAME)

Mo

IT 75-91-2P, Tert-Butyl hydroperoxide  
RL: **IMP (Industrial manufacture)**; **PUR (Purification or recovery)**; **RCT (Reactant)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**  
(process for recovering propylene and isobutane by tert-Bu alc. absorption in oxidation of isobutane and epoxidn. of propylene)  
RN 75-91-2 CAPLUS  
CN Hydroperoxide, 1,1-dimethylethyl (9CI) (CA INDEX NAME)

HO-O-Bu-t

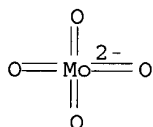
IT 7782-44-7, Oxygen, reactions  
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**  
(process for recovering propylene and isobutane by tert-Bu alc. absorption in oxidation of isobutane and epoxidn. of propylene)  
RN 7782-44-7 CAPLUS  
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

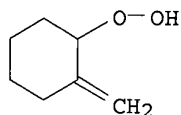
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 59 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1998:115291 CAPLUS  
DOCUMENT NUMBER: 128:179971  
TITLE: Heterogeneous molybdate catalysts for the generation of singlet molecular oxygen (1Δg) from H2O2  
AUTHOR(S): van Laar, F.; De Vos, D.; Vanoppen, D.; Sels, B.; Jacobs, P. A.; Del Guerzo, A.; Pierard, F.; Kirsh-De

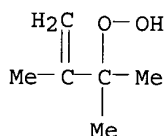
CORPORATE SOURCE: Mesmaeker, A.  
 Center Surface Science and Catalysis, K. U. Leuven,  
 Heverlee, B-3001, Belg.  
 SOURCE: Chemical Communications (Cambridge) (1998), (2),  
 267-268  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The immobilization of molybdate on Mg,Al-LDH (layered double hydroxide)  
 leads to an active, heterogeneous catalyst that generates singlet mol.  
 oxygen from hydrogen peroxide in the absence of soluble base.  
 α-Terpinene, 1-methylcyclohexene, and 2,3-dimethyl-2-butene were  
 subjected to (per)oxidation by the immobilized molybdate.  
 IT **14259-85-9**  
 RL: **CAT (Catalyst use); USES (Uses)**  
 (heterogeneous molybdate **catalysts** for generation of singlet  
 mol. oxygen from H<sub>2</sub>O<sub>2</sub>)  
 RN 14259-85-9 CAPLUS  
 CN Molybdate (MoO<sub>4</sub><sup>2-</sup>), (T-4)- (9CI) (CA INDEX NAME)



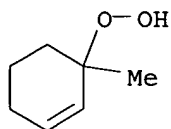
IT **4065-78-5P**, Hydroperoxide, 2-methylenecyclohexyl  
**13249-73-5P**, Hydroperoxide, 1,1,2-trimethyl-2-propenyl  
**18428-16-5P**, Hydroperoxide, 1-methyl-2-cyclohexen-1-yl  
**56595-78-9P**, Hydroperoxide, 2-methyl-2-cyclohexen-1-yl  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (heterogeneous molybdate catalysts for generation of singlet mol.  
 oxygen from H<sub>2</sub>O<sub>2</sub>)  
 RN 4065-78-5 CAPLUS  
 CN Hydroperoxide, 2-methylenecyclohexyl (7CI, 8CI, 9CI) (CA INDEX NAME)



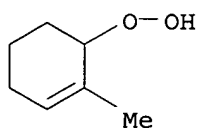
RN 13249-73-5 CAPLUS  
 CN Hydroperoxide, 1,1,2-trimethyl-2-propenyl (9CI) (CA INDEX NAME)



RN 18428-16-5 CAPLUS  
 CN Hydroperoxide, 1-methyl-2-cyclohexen-1-yl (8CI, 9CI) (CA INDEX NAME)



RN 56595-78-9 CAPLUS  
 CN Hydroperoxide, 2-methyl-2-cyclohexen-1-yl (9CI) (CA INDEX NAME)



IT 7782-44-7P, Oxygen, preparation  
 RL: PNU (Preparation, unclassified); RCT (Reactant); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (singlet; heterogeneous molybdate catalysts for generation of singlet  
 mol. oxygen from H2O2)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 60 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1997:424747 CAPLUS  
 DOCUMENT NUMBER: 127:33911  
 TITLE: Preparation of mixtures of cycloalkyl hydroperoxides,  
 cycloalkanols, and cycloalkanones  
 INVENTOR(S): Ninomiya, Kohei; Yamamoto, Tomohiko; Umiiso, Koji;  
 Kawai, Joji; Naito, Tatsuya  
 PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09143109	A2	19970603	JP 1995-309102	19951128

## PRIORITY APPLN. INFO.:

JP 1995-309102

19951128

AB Title mixts., useful as materials for polyamides, intermediates for chems., and organic solvents (no data), are prepared by oxidation of cycloalkanes

by mol. O in the presence of Co compds. and N-hydroxydicarboximides. Cyclohexane was treated with O in the presence of N-hydroxyphthalimide and Co octylate at 160° under 10 kg/cm<sup>2</sup>G for 0.5 h to give cyclohexyl hydroperoxide, cyclohexanol, and cyclohexanone with 45.6, 26.8, and 16.4% selectivity, resp., at 3.7% conversion.

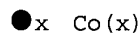
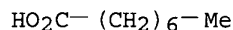
IT 6700-85-2 21679-46-9, Cobalt tris(acetylacetonate)

RL: CAT (Catalyst use); USES (Uses)

(preparation of mixts. of cycloalkyl hydroperoxides, cycloalkanols, and cycloalkanones by oxidation of cycloalkanes with Co compds. and hydroxydicarboximides)

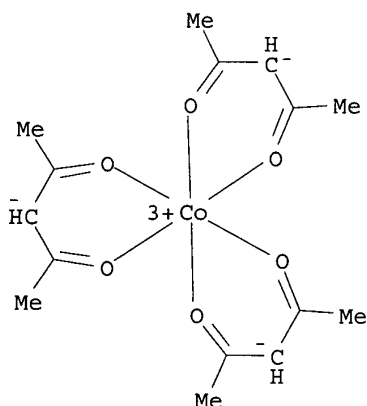
RN 6700-85-2 CAPLUS

CN Octanoic acid, cobalt salt (8CI, 9CI) (CA INDEX NAME)



RN 21679-46-9 CAPLUS

CN Cobalt, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI)  
(CA INDEX NAME)



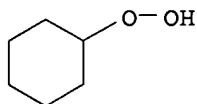
IT 766-07-4P, Cyclohexyl hydroperoxide

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of mixts. of cycloalkyl hydroperoxides, cycloalkanols, and cycloalkanones by oxidation of cycloalkanes with Co compds. and hydroxydicarboximides)

RN 766-07-4 CAPLUS

CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of mixts. of cycloalkyl hydroperoxides, cycloalkanols, and cycloalkanones by oxidation of cycloalkanes with Co compds. and hydroxydicarboximides)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 61 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:320710 CAPLUS

DOCUMENT NUMBER: 126:293181

TITLE: Method for producing arylalkyl hydroperoxides

INVENTOR(S): Matsui, Narikazu; Fujita, Terunori

PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

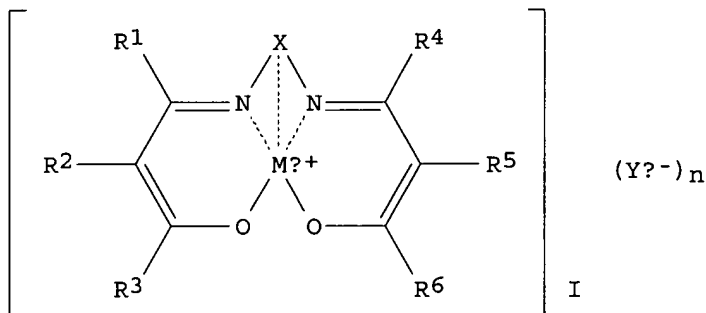
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 09067338	A2	19970311	JP 1995-222361	19950830
PRIORITY APPLN. INFO.:			JP 1995-222361	19950830
OTHER SOURCE(S):		CASREACT 126:293181; MARPAT 126:293181		
GI				



- AB Arylalkyl hydroperoxides represented by formula  $\text{Ar}[\text{C}(\text{P})(\text{Q})\text{OOH}]_x$  (P, Q = H, alkyl;  $x = 1-3$ ; Ar = x-valent aromatic hydrocarbon group) are prepared by oxidation of arylalkyl hydrocarbons  $\text{Ar}[\text{C}(\text{P})(\text{Q})\text{H}]_x$  (P, Q,  $x =$  same as above) with an gas containing oxygen in the presence of a transition metal complex (e.g. I; M = transition metal having +a valences; X = atom having a lone pair electrons and forming a partial structure of a ligand together with 2 nitrogen atoms coordinating to the central metal ion; R1 - R6 = H, halo, organic group, each group being optionally linked to the adjacent organic group or forming a ring together with the adjacent organic group; Y = counter ion of -b valences;  $a = 2+nb$ , wherein  $2 \leq a \leq 5$  and  $n = 0-3$ ). Preferably the transition metal complex is N,N'-bis(1-methyl-3-oxobutylidene)-4-aza-1,7-heptanediamine- or N,N'-disalicylidene-4-aza-1,7-heptanediamine-transition metal complex. The transition metal is selected from Mn, Co, Cu, Ni, Fe, Ta, Zr, Rh, Ru, and ions. This process uses a transition metal complex containing electron-donating atoms, i.e. N and O together with atoms selected from N, O, S, and P having lone pair electrons, and converts arylalkyl hydrocarbons into arylalkyl hydroperoxides of high concentration in high selectivity and high reaction rate using a small amount of the catalyst. Thus, 2 mg N,N'-bis(1-methyl-3-oxobutylidene)-4-aza-1,7-heptanediamine-cobalt complex was added to a mixture of 90 g cumene and 10 g cumene hydroperoxide, dissolved, and heated to 80°, followed by blowing air at 180 mL/min into the solution for 6 h to give cumene hydroperoxide at 3.1 weight%/h with 84 mol% selectivity.
- IT 7439-89-6D, Iron, complexes, uses 7440-47-3D, Chromium, complexes, uses 14167-18-1, [N,N'-Disalicylideneethylenediamine]cobalt 14167-20-5, [N,N'-Disalicylideneethylenediamine]nickel 15137-09-4 33916-81-3 66328-14-1 70335-48-7 189134-24-5 189134-25-6  
 RL: CAT (Catalyst use); USES (Uses)  
 (preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)
- RN 7439-89-6 CAPLUS  
 CN Iron (7CI, 8CI, 9CI) (CA INDEX NAME)

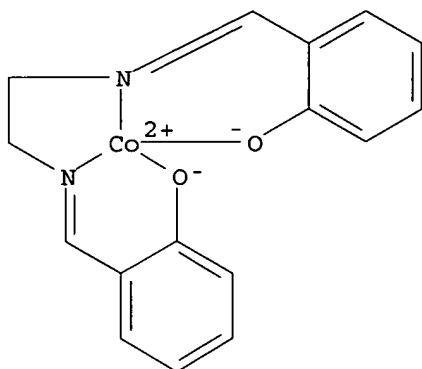
Fe

- RN 7440-47-3 CAPLUS  
 CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

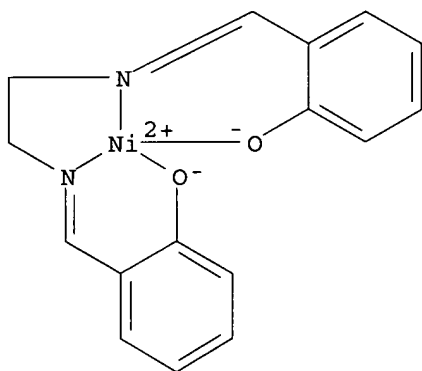
- RN 14167-18-1 CAPLUS  
 CN Cobalt, [[2,2'-(1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[pheno lato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)





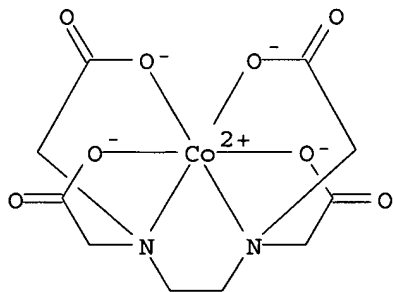
RN 14167-20-5 CAPLUS

CN Nickel, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]-, (SP-4-2)-(9CI) (CA INDEX NAME)



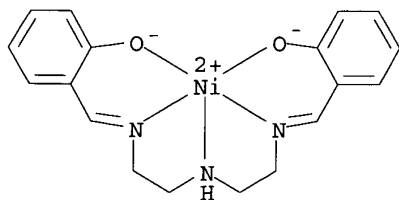
RN 15137-09-4 CAPLUS

CN Cobaltate(2-), [[N,N'-1,2-ethanediylbis[N-[(carboxy-κO)methyl]glycinato-κN,κO]](4-)]-, disodium, (OC-6-21)-(9CI) (CA INDEX NAME)

● 2 Na<sup>+</sup>

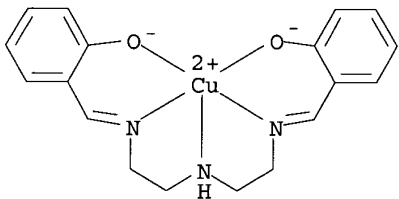
RN 33916-81-3 CAPLUS

CN Nickel, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]- (9CI) (CA INDEX NAME)



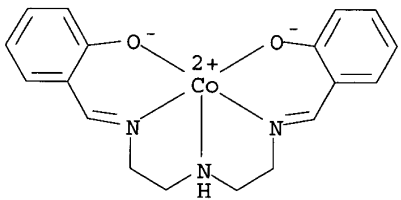
RN 66328-14-1 CAPLUS

CN Copper, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]- (9CI) (CA INDEX NAME)



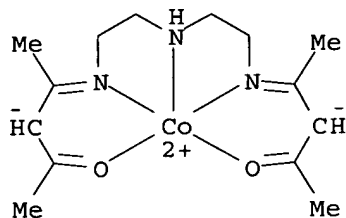
RN 70335-48-7 CAPLUS

CN Cobalt, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]-, (SP-5-32)- (9CI) (CA INDEX NAME)



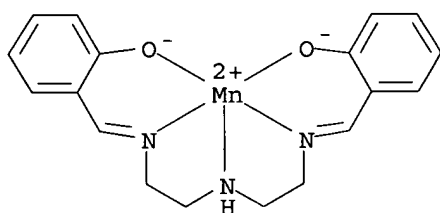
RN 189134-24-5 CAPLUS

CN Cobalt, [[4,4'-[(imino-κN)bis(2,1-ethanediylnitrilo-κN)]bis[2-pentanonato-κO]](2-)]- (9CI) (CA INDEX NAME)



RN 189134-25-6 CAPLUS

CN Manganese, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]- (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



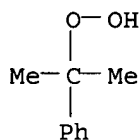
IT 80-15-9P, Cumene hydroperoxide

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L34 ANSWER 62 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1997:320709 CAPLUS

DOCUMENT NUMBER: 126:293180  
 TITLE: Method for producing arylalkyl hydroperoxides  
 INVENTOR(S): Kagayama, Akishi; Fujita, Terunori  
 PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09067337	A2	19970311	JP 1995-222360	19950830
PRIORITY APPLN. INFO.:			JP 1995-222360	19950830

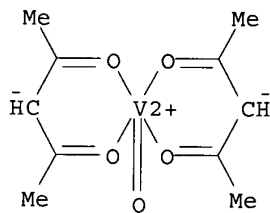
OTHER SOURCE(S): CASREACT 126:293180; MARPAT 126:293180

AB Arylalkyl hydroperoxides represented by formula  $\text{Ar}[\text{C}(\text{P})(\text{Q})\text{OOH}]_n$  (P, Q = H, alkyl; n = 1-3; Ar = n-valent aromatic hydrocarbon group) are prepared by oxidation of arylalkyl hydrocarbons  $\text{Ar}[\text{C}(\text{P})(\text{Q})\text{H}]_n$  (P, Q, n = same as above) with an gas containing oxygen in the presence of an oxometal compound. The oxometal compds. are represented by formula  $\text{M}(\text{:O})\text{L}_n$  (M = metal; L = ligand; n = 1-8), which are preferably oxovanadium, oxotitanium, and oxozirconium compds. This process uses an oxometal compound which allows oxidation reaction at a .apprx.80° temperature range at a practical reaction rate and converts arylalkyl hydrocarbons into arylalkyl hydroperoxides of high concentration in high selectivity. Thus, 2 mg oxotitanium(II) acetylacetonate was added to a mixture of 90 g cumene and 10 g cumene hydroperoxide, and heated to 80°, followed by blowing air at 180 mL/min into the mixture for 6 h with stirring to give cumene hydroperoxide at 1.1 weight%/h and final concentration 16.9 weight% with 91 mol% selectivity.

IT 3153-26-2, Oxovanadium(II) acetylacetonate **7440-62-2D**, Vanadium, 1,4,8,11-Tetraazacyclotetradecane complexes, uses  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)

RN 3153-26-2 CAPLUS

CN Vanadium, oxobis(2,4-pentanedionato-κO,κO')-, (SP-5-21)- (9CI)  
 (CA INDEX NAME)



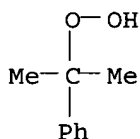
RN 7440-62-2 CAPLUS

CN Vanadium (8CI, 9CI) (CA INDEX NAME)

IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of oxometal compound metal complexes)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 80-15-9P, Cumene hydroperoxide  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of oxometal compound metal complexes)  
 RN 80-15-9 CAPLUS  
 CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L34 ANSWER 63 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:198217 CAPLUS

DOCUMENT NUMBER: 126:277162

TITLE: Oxidations by the reagent O<sub>2</sub>-H<sub>2</sub>O<sub>2</sub>-vanadium complex-pyrazine-2-carboxylic acid. 8. Efficient oxygenation of methane and other lower alkanes in acetonitrile

AUTHOR(S): Nizova, Galina V.; Suss-Fink, Georg; Shul'pin, Georgiy B.

CORPORATE SOURCE: Semenov Inst. Chemical Physics, Russian Academy Sciences, Moscow, 117977, Russia

SOURCE: Tetrahedron (1997), 53(10), 3603-3614

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 126:277162

AB All 5 C<sub>1</sub>-C<sub>4</sub> alkanes were readily oxidized in MeCN by air and H<sub>2</sub>O<sub>2</sub> at 20-75° using the catalytic system (n-Bu<sub>4</sub>N)VO<sub>3</sub>-pyrazine-2-carboxylic acid. Apart from alkyl hydroperoxides which are the primary oxidation products, more stable derivs. (alcs., aldehydes or ketones, and carboxylic acids) are obtained with high total turnover nos. (e.g., 420 for CH<sub>4</sub> and 2130 for C<sub>2</sub>H<sub>6</sub> at 75° after 4 h). In the case of ethane and cyclohexane (I), alkanes do not yield oxygenated products in the absence of air. I oxidation under 18O<sub>2</sub> showed a high degree of 18O incorporation into the oxygenated products. Thus, H<sub>2</sub>O<sub>2</sub> is only a promoter while O<sub>2</sub> is the true oxidant in this oxidation

IT 76060-16-7, Tetrabutylammonium trioxovanadate(-1)

RL: CAT (Catalyst use); USES (Uses)

(efficient oxidation of lower alkanes in acetonitrile by oxygen-hydrogen

peroxide-vanadium complex-pyrazinecarboxylic acid reagent)

RN 76060-16-7 CAPLUS

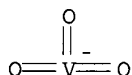
CN 1-Butanaminium, N,N,N-tributyl-, trioxovanadate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 13981-20-9

CMF 03 V

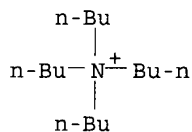
CCI CCS



CM 2

CRN 10549-76-5

CMF C16 H36 N



IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(efficient oxidation of lower alkanes in acetonitrile by oxygen-hydrogen peroxide-vanadium complex-pyrazinecarboxylic acid reagent)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 75-91-2P 3031-73-0P, Methyl hydroperoxide

3031-74-1P, Ethyl hydroperoxide 3031-75-2P,

Hydroperoxide, 1-methylethyl 4813-50-7P, Butyl hydroperoxide

5618-63-3P, Isobutyl hydroperoxide 6068-96-8P,

Hydroperoxide, propyl 13020-06-9P, sec-Butyl hydroperoxide

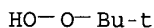
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

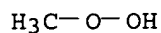
(efficient oxidation of lower alkanes in acetonitrile by oxygen-hydrogen peroxide-vanadium complex-pyrazinecarboxylic acid reagent)

RN 75-91-2 CAPLUS

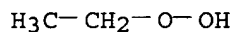
CN Hydroperoxide, 1,1-dimethylethyl (9CI) (CA INDEX NAME)



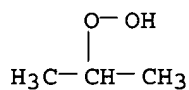
RN 3031-73-0 CAPLUS  
CN Hydroperoxide, methyl (9CI) (CA INDEX NAME)



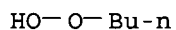
RN 3031-74-1 CAPLUS  
CN Hydroperoxide, ethyl (9CI) (CA INDEX NAME)



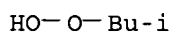
RN 3031-75-2 CAPLUS  
CN Hydroperoxide, 1-methylethyl (9CI) (CA INDEX NAME)



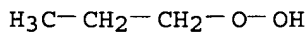
RN 4813-50-7 CAPLUS  
CN Hydroperoxide, butyl (9CI) (CA INDEX NAME)



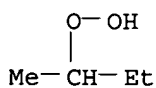
RN 5618-63-3 CAPLUS  
CN Hydroperoxide, 2-methylpropyl (9CI) (CA INDEX NAME)



RN 6068-96-8 CAPLUS  
CN Hydroperoxide, propyl (9CI) (CA INDEX NAME)



RN 13020-06-9 CAPLUS  
CN Hydroperoxide, 1-methylpropyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 64 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:138298 CAPLUS

DOCUMENT NUMBER: 126:237966

TITLE: Olefin oxidation by the system H<sub>2</sub>O<sub>2</sub>/MoO<sub>4</sub><sup>2-</sup>: competition between epoxidation and peroxidation

AUTHOR(S): Nardello, Veronique; Bouttemy, Sabine; Aubry, Jean-Marie

CORPORATE SOURCE: Equipe de Recherches sur les Radicaux Libres et l'Oxygene Singulet, URA CNRS 351, Faculte de Pharmacie de Lille, BP 83, Lille, F-59006, Fr.

SOURCE: Journal of Molecular Catalysis A: Chemical (1997), 117(1-3, Proceedings of the 6th International Symposium on the Activation of Dioxygen and Homogeneous Catalytic Oxidation, 1996), 439-447  
CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A symposium. The oxidation of tiglic acid by the catalytic system hydrogen peroxide/molybdate ions is investigated in water under varying conditions of pH. Using similar conditions of temperature and concns., we show that two different reaction pathways compete leading either to an epoxide in acidic medium or to an allylic hydroperoxide in alkaline medium. These results are interpreted in terms of the involvement of two peroxomolybdates. Epoxidn. probably proceeds via the tetraperoxodimolybdate Mo<sub>2</sub>O<sub>3</sub>(O<sub>2</sub>)<sub>4</sub><sup>2-</sup> whereas peroxidn. involves singlet oxygen, <sup>1</sup>O<sub>2</sub>, (<sup>1</sup>Δg), formed as a result of the decomposition of the triperoxomolybdate MoO(O<sub>2</sub>)<sub>3</sub><sup>2-</sup>. Finally, exptl. conditions are given to obtain selectively the epoxide or the hydroperoxide.

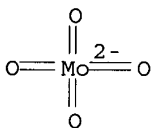
IT 7631-95-0, Sodium molybdate 13446-49-6, Potassium molybdate

RL: CAT (Catalyst use); USES (Uses)

(epoxidn. and peroxidn. of olefins by H<sub>2</sub>O<sub>2</sub>/MoO<sub>4</sub><sup>2-</sup>)

RN 7631-95-0 CAPLUS

CN Molybdate (MoO<sub>4</sub><sup>2-</sup>), disodium, (T-4)- (9CI) (CA INDEX NAME)

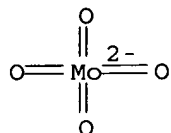


● 2 Na<sup>+</sup>

RN 13446-49-6 CAPLUS

CN Molybdate (MoO<sub>4</sub><sup>2-</sup>), dipotassium, (T-4)- (9CI) (CA INDEX NAME)



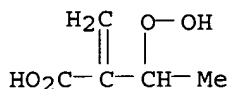
● 2 K<sup>+</sup>

IT 99268-55-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(epoxidn. and peroxidn. of olefins by H<sub>2</sub>O<sub>2</sub>/MoO<sub>4</sub><sup>2-</sup>)

RN 99268-55-0 CAPLUS

CN Butanoic acid, 3-hydroperoxy-2-methylene- (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions

RL: FMU (Formation, unclassified); RCT (Reactant); FORM  
(Formation, nonpreparative); RACT (Reactant or reagent)  
(peroxidn. of olefins by singlet oxygen formed from H<sub>2</sub>O<sub>2</sub>/MoO<sub>4</sub><sup>2-</sup>)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 65 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:218953 CAPLUS

DOCUMENT NUMBER: 127:4776

TITLE: Iron oxide colloids and t-butyl hydroperoxide in  
reverse microemulsions: a new and efficient system for  
carbon-hydrogen bond activation

AUTHOR(S): Launay, F.; Patin, H.

CORPORATE SOURCE: Lab. Chim. Organ. Substances Naturelles, CNRS URA,  
Rennes, 35700, Fr.SOURCE: New Journal of Chemistry (1997), 21(2), 247-256  
CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Gauthier-Villars

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Iron oxide colloids generated by the hydrolysis of ferric nitrate  
nonahydrate in Aerosol-OT reverse microemulsions catalyze (after the addition  
of tert-Bu hydroperoxide) the functionalization of the hydrocarbons  
constituting the continuous phase of these micellar systems. In the case  
of cyclooctane, used to set up this new model and in all the preliminary

studies, the carbon-hydrogen bond activation products are (in decreasing order) tert-butylperoxycyclooctane, cyclooctene, cyclooctanone and cyclooctanol, under static nitrogen atmospheric and at room temperature This reaction

is very sensitive to temperature variations and dioxygen partial pressure. Cycloalkane tert-Bu peroxidn. remains the major process at 50°C under anaerobic conditions and makes this procedure an interesting alternative to other methods already described in the literature. The evolvement of cyclooctane oxidation into an autoxidn. reaction in the presence of mol. oxygen and model extension expts. to other substrates gave the following sequence of regioselectivity:  $3^\circ > 2^\circ > 1^\circ$ , in agreement with an homolytic cleavage of C-H bonds. The nature of the active species in such a dispersed medium is discussed on the basis of recently published results dealing with the influence of solvent polarity on tBHP decomposition

IT 1317-60-8, Hematite, uses

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)

(colloidal  $\alpha$ -; iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)

RN 1317-60-8 CAPLUS

CN Hematite (Fe<sub>2</sub>O<sub>3</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====	=====	=====
O	3	17778-80-2
Fe	2	7439-89-6

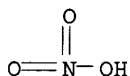
IT 7782-61-8, Ferric nitrate nonahydrate 10421-48-4, Ferric nitrate

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)

RN 7782-61-8 CAPLUS

CN Nitric acid, iron(3+) salt, nonahydrate (9CI) (CA INDEX NAME)

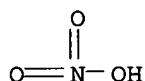


● 1/3 Fe(III)

● 3 H<sub>2</sub>O

RN 10421-48-4 CAPLUS

CN Nitric acid, iron(3+) salt (8CI, 9CI) (CA INDEX NAME)



● 1/3 Fe(III)

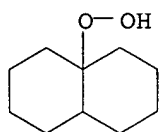
IT 4181-83-3P 5130-47-2P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)

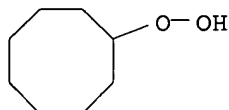
RN 4181-83-3 CAPLUS

CN Hydroperoxide, octahydro-4a(2H)-naphthalenyl (9CI) (CA INDEX NAME)



RN 5130-47-2 CAPLUS

CN Hydroperoxide, cyclooctyl (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions

RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**; USES (Uses)

(radical trap; iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 98 THERE ARE 98 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 66 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:133466 CAPLUS

DOCUMENT NUMBER: 126:224918

TITLE: Oxygen activation by metal complexes and alkyl

hydroperoxides. Applications of mechanistic probes to explore the role of alkoxyl radicals in alkane functionalization

AUTHOR(S): MacFaul, Philip A.; Arends, Isabella W. C. E.; Ingold, Keith U.; Wayner, Danial D. M.

CORPORATE SOURCE: Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON, K1A 0R6, Can.

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1997), (2), 135-145  
CODEN: JCPKBH; ISSN: 0300-9580

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The mechanism of the oxidation of cycloalkanes by tertiary alkyl hydroperoxides catalyzed by iron(III) dichlorotris(2-pyridylmethyl)amine [FeIIICl<sub>2</sub>(TPA)]<sup>+</sup> and by the acetate bridged ( $\mu$ -oxo) di-iron complex [Fe<sub>2</sub>III(TPA)<sub>2</sub>O(OAc)]<sub>3</sub><sup>+</sup> has been investigated. Product studies do not support oxidation via a high valent iron-oxo intermediate (formally FeV:O), but are consistent with a mechanism involving hydrogen atom abstraction from the alkane by alkoxyl radicals derived from the hydroperoxide. In the presence of a large excess of tert-Bu hydroperoxide, the oxidation of cyclohexane yields cyclohexanone, cyclohexanol and tert-Bu cyclohexyl peroxide in more than stoichiometric amts. and, in the case of the mono-iron catalyst, one equivalent of cyclohexyl chloride. Replacement of Me<sub>3</sub>COOH by hydroperoxides which could yield tert-alkoxyl radicals having much shorter lifetimes than the tert-butoxyl radical prevents oxidation of the cycloalkane. The products obtained with these hydroperoxide mechanistic probes are those derived from the fast unimol. reactions (generally  $\beta$ -scissions) of the corresponding alkoxyl radicals. The inapplicability of di-Me sulfide as a mechanistically diagnostic trap for the putative FeV:O intermediate and the value of di-tert-Bu hyponitrite as a non-iron-based source of tert-butoxyl radicals are discussed.

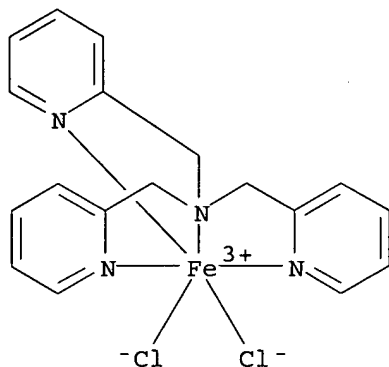
IT 128412-29-3 164223-84-1 188175-48-6  
RL: CAT (Catalyst use); USES (Uses)  
(mechanism of the oxidation of cycloalkanes by tertiary alkyl hydroperoxides catalyzed by iron(III) complexes)

RN 128412-29-3 CAPLUS

CN Iron(1+), [N,N-bis[(2-pyridinyl- $\kappa$ N)methyl]-2-pyridinemethanamine- $\kappa$ N1, $\kappa$ N2]dichloro-, (OC-6-32)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

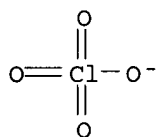
CRN 128412-28-2  
CMF C18 H18 Cl2 Fe N4  
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 164223-84-1 CAPLUS

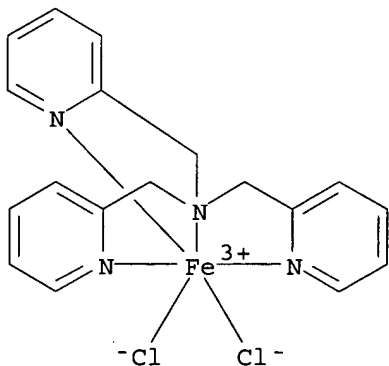
CN Iron(1+), [N,N-bis[(2-pyridinyl-κN)methyl]-2-pyridinemethanamine-κN1,κN2]dichloro-, (OC-6-32)-, tetrafluoroborate(1-) (9CI)  
(CA INDEX NAME)

CM 1

CRN 128412-28-2

CMF C18 H18 Cl2 Fe N4

CCI CCS

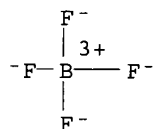


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



RN 188175-48-6 CAPLUS

CN Iron(3+), [ $\mu$ -(acetato- $\kappa\text{O}:\kappa\text{O}'$ )]bis[N,N-bis[(2-pyridinyl- $\kappa\text{N}$ )methyl]-2-pyridinemethanamine- $\kappa\text{N1},\kappa\text{N2}$ ]- $\mu$ -oxodi-, stereoisomer, tris[tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

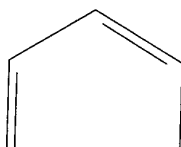
CM 1

CRN 121757-78-6

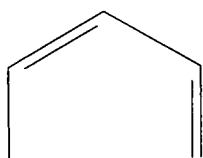
CMF C38 H39 Fe2 N8 O3

CCI CCS

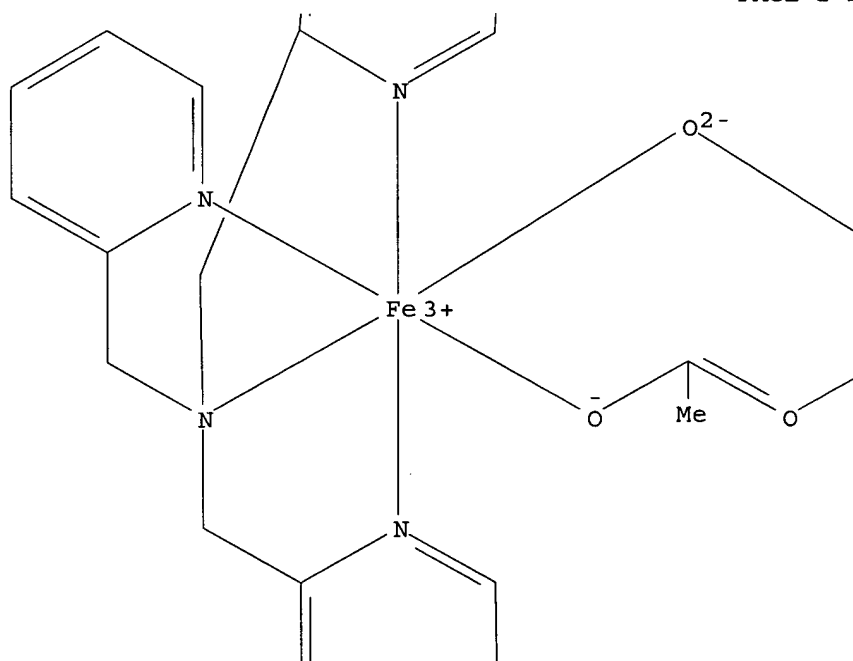
PAGE 1-A



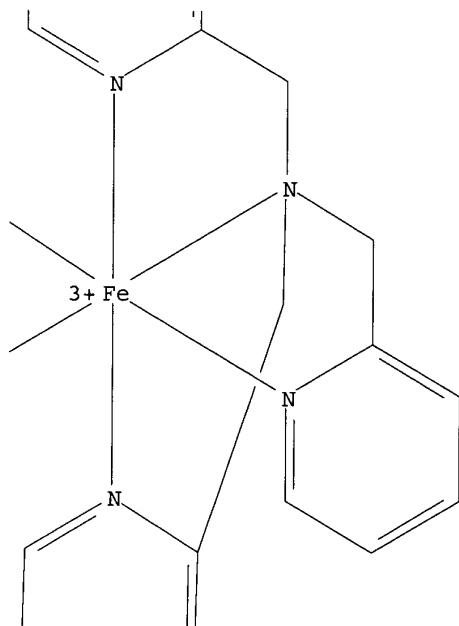
PAGE 1-B



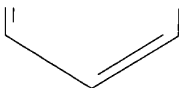
PAGE 2-A



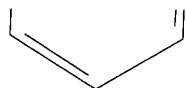
PAGE 2-B



PAGE 3-A



PAGE 3-B



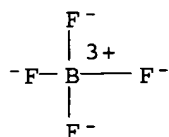
CM 2

CRN 14874-70-5

CMF B F4

CCI CCS

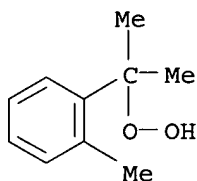




IT 7782-44-7, Oxygen, reactions  
 RL: PEP (Physical, engineering or chemical process); RCT  
 (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (mechanism of the oxidation of cycloalkanes by tertiary alkyl  
 hydroperoxides catalyzed by iron(III) complexes)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 13387-56-9P, o-Methylcumene hydroperoxide  
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant);  
 SPN (Synthetic preparation); PREP (Preparation); PROC  
 (Process); RACT (Reactant or reagent)  
 (mechanism of the oxidation of cycloalkanes by tertiary alkyl  
 hydroperoxides catalyzed by iron(III) complexes)  
 RN 13387-56-9 CAPLUS  
 CN Hydroperoxide, 1-methyl-1-(2-methylphenyl)ethyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 101 THERE ARE 101 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L34 ANSWER 67 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:603937 CAPLUS  
 DOCUMENT NUMBER: 123:111661  
 TITLE: Process for production of cresols via oxygenation of  
 cymene and selective removal of cymene primary  
 hydroperoxide  
 INVENTOR(S): Ikimi, Kiyoshi; Ikeda, Yoichi; Murakami, Akira;  
 Okamoto, Kazushige; Tokumaru, Tooru; Hazama, Motoo  
 PATENT ASSIGNEE(S): Suitomo Chemical Co., Ltd., Japan  
 SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 10,837,  
 abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5399791	A	19950321	US 1994-202160	19940225
JP 05208928	A2	19930820	JP 1992-16136	19920131
JP 3537455	B2	20040614		

PRIORITY APPLN. INFO.: JP 1992-16136 A 19920131  
US 1993-10837 B2 19930129

OTHER SOURCE(S): CASREACT 123:111661; MARPAT 123:111661

AB A process for the production of cresols, comprising the steps of: (a) conducting oxygenation of cymene with oxygen gas or an oxygen-containing gas without any addition of an alkali, thereby obtaining a solution of oxygenation products containing tertiary and primary hydroperoxides of cymene; (b) washing the solution of oxygenation products obtained in step (a) with an aqueous alkali solution at a temperature in the range of from 10° to 95°, said aqueous alkali solution having a concentration of 0.1 to 2.0 weight %, and the weight ratio of the aqueous alkali solution to the solution of oxygenation products being in the range of from 1/5 to 1/15 (weight/weight); (c) subjecting the solution of oxygenation products obtained in step (b) to hydrogenation at a temperature in the range of from 60° to 100° to decrease the content of primary hydroperoxide in such a manner that the weight ratio of primary hydroperoxide to tertiary hydroperoxide is not greater than 1/25 (weight/weight); (d) subjecting the solution treated in step (c) to decomposition in the presence of a catalyst; and (e) subjecting the solution treated in step (d) to hydrogenation to obtain cresols. Thus, e.g., oxidation of cymene (807.0 g; content, 99.3%) and a cymene solution [78.0 g; cymene content, 82.1%; tertiary hydroperoxide (3HPO) content, 11.2%; and 1HPO content, 0.65%] containing cymene hydroperoxide with air afforded 909.2 g of a hydroperoxide mixture-containing oil phase (composition: cymene, 81.9%; 3HPO, 12.1%; 1HPO, 2.2% + others); hydrogenation over 1% palladium-titania catalyst afforded 909.2 g of the reaction mixture (composition: cymene, 81.8%; 3HPO, 11.0%; 1HPO, 0.03% + others) in which the weight ratio of 1HPO to 3HPO is 1/370, and the degree of conversion is 98.7% for 1HPO and 8.7% for 3HPO, resp.; from this reaction mixture, the unreacted portion (699.8 g) of cymene is removed by distillation, 209.3 g of the concentrate is obtained (composition: cymene, 21.0%; 3HPO, 47.8%; 1HPO, 0.13%); decomposition of the mixture in presence of sulfuric acid (0.17 g) and acetone (29 g) afforded a 238.3 g solution of decomposition products (composition: cymene, 18.3%; 3HPO, not found; 1HPO, not found; cresol, 26.0%; + others) with the yield of cresol from consumed cymene = 59.4%; hydrogenation of decomposition products over 1% palladium-titania afforded 63.0 g of cresol and 82.1 g of cymene, with the yield of cresol from consumed cymene = 86%. When the first hydrogenation step was omitted, the yield of cresol from consumed cymene is 72.8%.

IT 7440-47-3, Chromium, uses 7440-50-8, Copper, uses  
RL: CAT (Catalyst use); USES (Uses)  
(copper-chromium catalysts; production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide)

RN 7440-47-3 CAPLUS  
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

RN 7440-50-8 CAPLUS  
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

IT 7440-02-0, Nickel, uses 7440-02-0D, Nickel,  
1,2-Diphenyl-1,2-ethenedithiol complexes 7440-50-8D, Copper,  
1,2-Diphenyl-1,2-ethenedithiol complexes 12026-57-2  
RL: CAT (Catalyst use); USES (Uses)  
(production of cresols via oxygenation of cymene and selective removal of  
cymene primary hydroperoxide)  
RN 7440-02-0 CAPLUS  
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-02-0 CAPLUS  
CN Nickel (8CI, 9CI) (CA INDEX NAME)

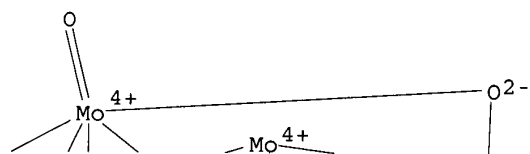
Ni

RN 7440-50-8 CAPLUS  
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

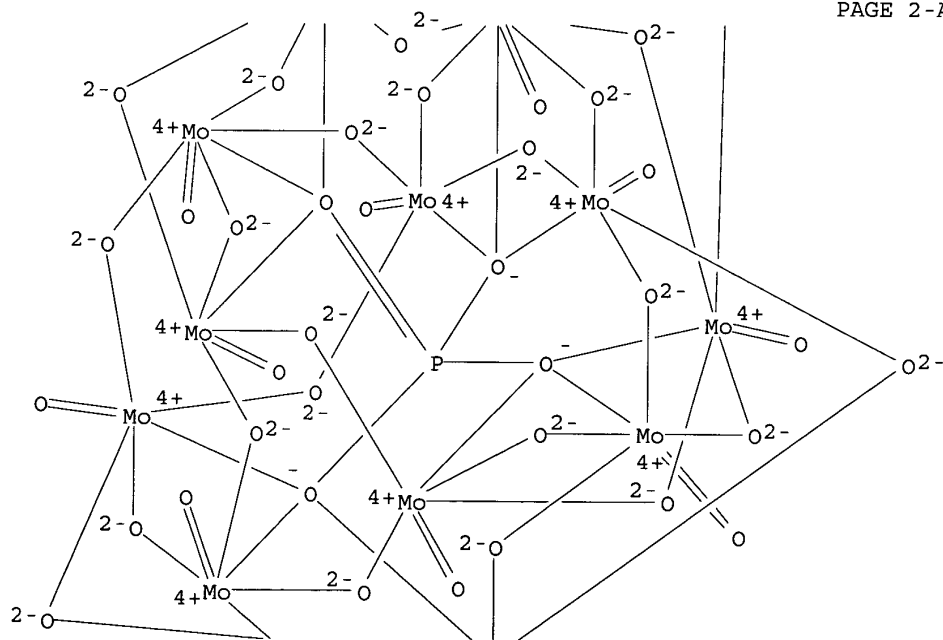
Cu

RN 12026-57-2 CAPLUS  
CN Molybdate(3-), tetracosam-oxododecaoxo[μ12-[phosphato(3-)-  
κO:κO:κO:κO':κO':κO':κO'':.kappa  
.O':κO':κO':κO':κO'']]dodeca-, trihydrogen  
(9CI) (CA INDEX NAME)

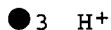
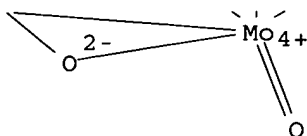
PAGE 1-A



PAGE 2-A



PAGE 3-A



IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 26444-17-7P, Cymene hydroperoxide

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

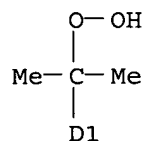
(production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide)

RN 26444-17-7 CAPLUS

CN Hydroperoxide, 1-methyl-1-(methylphenyl)ethyl (9CI) (CA INDEX NAME)



D1-Me



L34 ANSWER 68 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:606901 CAPLUS

DOCUMENT NUMBER: 123:9156

TITLE: Process and catalysts for producing aromatic  
peroxycarboxylic acids from aromatic aldehydes  
INVENTOR(S): Oda, Yoshiaki  
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan  
SOURCE: Eur. Pat. Appl., 6 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 653420	A1	19950517	EP 1994-117863	19941111
EP 653420	B1	19980311		
R: DE, FR, GB, IT, NL				
JP 07188161	A2	19950725	JP 1994-244284	19941007
US 5523468	A	19960604	US 1994-341901	19941115
PRIORITY APPLN. INFO.:			JP 1993-286607	A 19931116
			JP 1994-244284	A 19941007

OTHER SOURCE(S): CASREACT 123:9156

AB Aromatic peroxycarboxylic acids (e.g., PhCO<sub>2</sub>OH) are prepared in high yield, without significant product decomposition, by reacting an aromatic aldehyde (e.g.,

PhCHO) and O<sub>2</sub>(g) in the presence of ≥1 transition metal oxide(s), selected from Cr, Mn, Fe, Co, Ni, and Cu, in a solvent (e.g., C<sub>6</sub>H<sub>6</sub>).

IT 1308-06-1, Cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) 1308-38-9, Chromium oxide (Cr<sub>2</sub>O<sub>3</sub>), uses 1309-37-1, Ferric oxide, uses 1313-13-9, Manganese IV oxide, uses 1314-06-3, Nickel oxide (Ni<sub>2</sub>O<sub>3</sub>) 1317-38-0, Cupric oxide, uses 1317-39-1, Cuprous oxide, uses 1317-61-9, Iron oxide (Fe<sub>3</sub>O<sub>4</sub>), uses 1345-25-1, Ferrous oxide, uses 7439-89-6D, Iron, oxides 7439-96-5D, Manganese, oxides 7440-02-0D, Nickel, oxides 7440-47-3D, Chromium, oxides 7440-48-4D, Cobalt, oxides 7440-50-8D, Copper, oxides

RL: CAT (Catalyst use); USES (Uses)

(catalysts for producing aromatic peroxycarboxylic acids from aromatic aldehydes)

RN 1308-06-1 CAPLUS

CN Cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 1308-38-9 CAPLUS

CN Chromium oxide (Cr<sub>2</sub>O<sub>3</sub>) (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 1309-37-1 CAPLUS

CN Iron oxide (Fe<sub>2</sub>O<sub>3</sub>) (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 1313-13-9 CAPLUS

CN Manganese oxide (MnO<sub>2</sub>) (8CI, 9CI) (CA INDEX NAME)



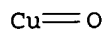
RN 1314-06-3 CAPLUS

CN Nickel oxide (Ni2O3) (6CI, 8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

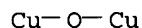
RN 1317-38-0 CAPLUS

CN Copper oxide (CuO) (8CI, 9CI) (CA INDEX NAME)



RN 1317-39-1 CAPLUS

CN Copper oxide (Cu2O) (8CI, 9CI) (CA INDEX NAME)



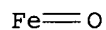
RN 1317-61-9 CAPLUS

CN Iron oxide (Fe3O4) (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 1345-25-1 CAPLUS

CN Iron oxide (FeO) (8CI, 9CI) (CA INDEX NAME)



RN 7439-89-6 CAPLUS

CN Iron (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 7439-96-5 CAPLUS

CN Manganese (8CI, 9CI) (CA INDEX NAME)



RN 7440-02-0 CAPLUS

CN Nickel (8CI, 9CI) (CA INDEX NAME)



RN 7440-47-3 CAPLUS

CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

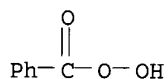
RN 7440-48-4 CAPLUS  
 CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

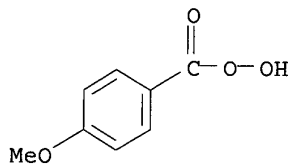
RN 7440-50-8 CAPLUS  
 CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

IT **93-59-4P**, Peroxybenzoic acid **940-10-3P**,  
 4-Methoxyperoxybenzoic acid **123088-67-5P**, Benzenecarboperoxoic  
 acid, 2,4-Dimethyl-  
 RL: **IMF (Industrial manufacture)**; **SPN (Synthetic**  
**preparation)**; **PREP (Preparation)**  
 (process and catalysts for producing aromatic peroxydicarboxylic acids from  
 aromatic aldehydes)  
 RN 93-59-4 CAPLUS  
 CN Benzenecarboperoxoic acid (9CI) (CA INDEX NAME)

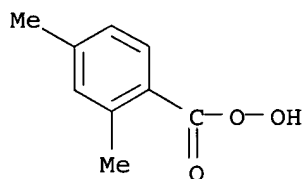


RN 940-10-3 CAPLUS  
 CN Benzenecarboperoxoic acid, 4-methoxy- (9CI) (CA INDEX NAME)



RN 123088-67-5 CAPLUS  
 CN Benzenecarboperoxoic acid, 2,4-dimethyl- (9CI) (CA INDEX NAME)





IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(process and catalysts for producing aromatic peroxycarboxylic acids from aromatic aldehydes)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

L34 ANSWER 69 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:988670 CAPLUS

DOCUMENT NUMBER: 124:175160

TITLE: Iron(II)-Induced Activation of Dioxygen for Oxygenation of Cyclohexene and Methyl Linoleate and Initiation of the Autoxidation of 1,4-Cyclohexadiene

AUTHOR(S): Hage, John P.; Powell, John A.; Sawyer, Donald T.

CORPORATE SOURCE: Department of Chemistry, Texas A and M University, College Station, TX, 77843-3255, USA

SOURCE: Journal of the American Chemical Society (1995), 117(51), 12897-8

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB FeII(byp)22+ and FeII(OPPh3)42+ in MeCN catalytically activate O2 for the direct oxygenation of cyclohexene of Me linoleate. The FeII(byp)22+/O2/MeCN system initiated the autoxidn. of 1,4-cyclohexadiene and PhCHO.

IT 15552-69-9 47921-14-2

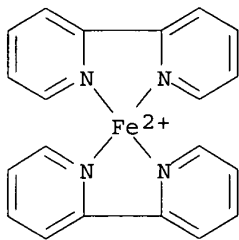
RL: CAT (Catalyst use); NUU (Other use, unclassified); USES

(Uses)

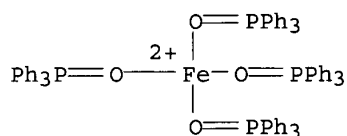
(iron(II)-induced activation of dioxygen for oxygenation of cyclohexene and Me linoleate)

RN 15552-69-9 CAPLUS

CN Iron(2+), bis(2,2'-bipyridine-κN1,κN1')- (9CI) (CA INDEX NAME)



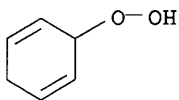
RN 47921-14-2 CAPLUS  
 CN Iron(2+), tetrakis(triphenylphosphine oxide-κO)-, (T-4)- (9CI) (CA INDEX NAME)



IT 7782-44-7, Dioxygen, reactions  
 RL: PEP (Physical, engineering or chemical process); RCT  
 (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (iron(II)-induced activation of dioxygen for oxygenation of cyclohexene  
 and Me linoleate)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



IT 173910-76-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (iron(II)-initiated autoxidn. of 1,4-cyclohexadiene and PhCHO)  
 RN 173910-76-4 CAPLUS  
 CN Hydroperoxide, 2,5-cyclohexadien-1-yl (9CI) (CA INDEX NAME)



L34 ANSWER 70 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1992:213711 CAPLUS  
 DOCUMENT NUMBER: 116:213711  
 TITLE: Carbon dioxide as modulator of the oxidative  
 properties of dioxygen in the presence of transition  
 metal systems

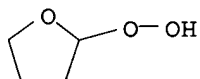
AUTHOR(S): Aresta, Michele; Fragale, Carlo; Quaranta, Eugenio;  
 Tommasi, Immacolata  
 CORPORATE SOURCE: Dip. Chim., CNR, Bari, 70126, Italy  
 SOURCE: Journal of the Chemical Society, Chemical  
 Communications (1992), (4), 315-17  
 CODEN: JCCCCAT; ISSN: 0022-4936  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 116:213711  
 AB In the presence of transition metal (Fe, Rh) catalysts, CO<sub>2</sub> can modulate  
 the oxidative properties of O<sub>2</sub> towards THF (THF) and styrene; the  
 intermediate formation of metal-peroxocarbonate species, seems to play a  
 key role in these processes. E.g., oxidation of THF by O<sub>2</sub> in the presence of  
 FeCl<sub>2</sub> gave 2-hydroxytetrahydrofuran (I), butyrolactone (II), succinic  
 anhydride, and succinaldehyde. Use of CO<sub>2</sub>-O<sub>2</sub> (1:1 by volume) gave I and II  
 selectively.  
 IT **7758-94-3**, Iron dichloride  
 RL: **CAT (Catalyst use)**; USES (Uses)  
 (catalyst, for oxidation of THF in presence of carbon dioxide)  
 RN 7758-94-3 CAPLUS  
 CN Iron chloride (FeCl<sub>2</sub>) (8CI, 9CI) (CA INDEX NAME)

Cl-Fe-Cl

IT **7782-44-7**, Oxygen, reactions  
 RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**  
 (oxidation by, of organic substrates, effect of carbon dioxide on)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT **4676-82-8P**  
 RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**  
 (preparation of, by oxidation of THF, catalytic)  
 RN 4676-82-8 CAPLUS  
 CN Hydroperoxide, tetrahydro-2-furanyl (9CI) (CA INDEX NAME)



L34 ANSWER 71 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1992:435485 CAPLUS  
 DOCUMENT NUMBER: 117:35485  
 TITLE: Application of air electrode  
 AUTHOR(S): Wu, Zhiyuan; Li, Shengxian  
 CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Wuhan, Peop. Rep. China  
 SOURCE: Wuhan Daxue Xuebao, Ziran Kexueban (1991), (3), 99-104

CODEN: WTHPDI; ISSN: 0253-9888

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Alkaline solution of hydrogen peroxide can be prepared by electroredn. of oxygen on

porous gas cathodes in caustic medium. The current efficiency and cathode lifetime depends on the condition of electrolysis. Exptl. results show that continuous operative lifetimes of the electrode can be longer than 2000 h at c.d. of 50 mA/cm<sup>2</sup>. The electrode is applied to preparation of oxygen by placing a MnO<sub>2</sub> covered iron screen in the cell. The number of coulombs required for generating same oxygen vols. is discussed.

IT 1308-06-1, Cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) 1313-13-9, Manganese dioxide, uses 12017-35-5, Cobalt nickel oxide (Co<sub>2</sub>NiO<sub>4</sub>)

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for decomposition of hydrogen peroxide)

RN 1308-06-1 CAPLUS

CN Cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) (8CI, 9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 1313-13-9 CAPLUS

CN Manganese oxide (MnO<sub>2</sub>) (8CI, 9CI) (CA INDEX NAME)



RN 12017-35-5 CAPLUS

CN Cobalt nickel oxide (Co<sub>2</sub>NiO<sub>4</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====+=====+=====		
O	4	17778-80-2
Co	2	7440-48-4
Ni	1	7440-02-0

IT 14691-59-9P, Peroxide (HO<sub>2</sub>-)

RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in electrochem. reduction of oxygen)

RN 14691-59-9 CAPLUS

CN Peroxide (HO<sub>2</sub>-) (8CI, 9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction of, electrochem., on porous gas electrode in alkaline medium, hydrogen peroxide production from)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 72 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:517196 CAPLUS

DOCUMENT NUMBER: 111:117196

TITLE: Catalytic oxidation of cyclohexene by oxygen

AUTHOR(S): Belov, P. S.; Nizova, S. A.; Fedorova, R. I.; Mitina, V. v.; Pleshivtseva, A. V.

CORPORATE SOURCE: Mosk. Inst. Nefti Gaza im Gubkina, Moscow, USSR

SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1989), 62(2), 353-7  
CODEN: ZPKHAB; ISSN: 0044-4618

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Selectivity of the oxidation of cyclohexene (I) by O to 1,2-epoxycyclohexane (II) and 2,3-epoxy-1-cyclohexanol (III) in the presence of the catalysts Cu(OAc)<sub>2</sub>, Co/zeolite, V<sub>2</sub> (a V-containing catalyst), VO(acac)<sub>2</sub> (acac = acetylacetonate), Mo(CO)<sub>6</sub>, and their mixts. was studied in an attempt to obtain II and III without introduction of cyclohexenyl hydroperoxide (IV) into the reaction mixture. I oxidation in the presence of Cu(OAc)<sub>2</sub>, Co/zeolite, or V<sub>2</sub> gave IV as the main product with II and III obtained in insignificant amts., whereas selectivity for II and III was relatively high with minor IV formation in oxidation in the presence of VO(acac)<sub>2</sub> or Mo(CO)<sub>6</sub>. The highest yields of II and III for binary catalyst systems were obtained by simultaneous introduction of V<sub>2</sub> and VO(acac)<sub>2</sub> into the reaction mixture at a 1:1 ratio. For ternary catalyst systems, the highest yields were obtained by I oxidation in the presence of 6:1:1 Co/zeolite-VO(acac)<sub>2</sub>-Mo(CO)<sub>6</sub> systems.

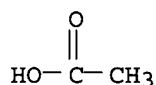
IT 142-71-2, Copper diacetate 3153-26-2,  
Oxobis(acetylacetonato)vanadium 7440-62-2, Vanadium, uses and  
miscellaneous 13939-06-5, Molybdenum hexacarbonyl

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for oxidation of cyclohexene to epoxycyclohexane and  
epoxycyclohexanol, selectivity of)

RN 142-71-2 CAPLUS

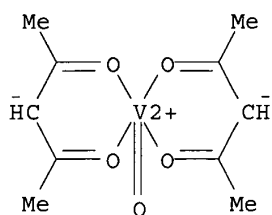
CN Acetic acid, copper(2+) salt (8CI, 9CI) (CA INDEX NAME)



● 1/2 Cu(II)

RN 3153-26-2 CAPLUS

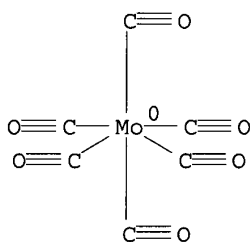
CN Vanadium, oxobis(2,4-pentanedionato-κO,κO')-, (SP-5-21)- (9CI)  
(CA INDEX NAME)



RN 7440-62-2 CAPLUS  
CN Vanadium (8CI, 9CI) (CA INDEX NAME)

V

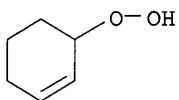
RN 13939-06-5 CAPLUS  
CN Molybdenum carbonyl ( $\text{Mo}(\text{CO})_6$ ), (OC-6-11) - (9CI) (CA INDEX NAME)



IT 7440-48-4, Cobalt, uses and miscellaneous  
RL: **CAT (Catalyst use)**; USES (Uses)  
(catalysts, zeolite-supported, for oxidation of cyclohexene to  
epoxycyclohexane and epoxycyclohexanol, selectivity of)  
RN 7440-48-4 CAPLUS  
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

IT 4845-05-0P  
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**  
(formation of, in cyclohexene oxidation to epoxycyclohexane and  
epoxycyclohexanol, effect of catalyst selectivity on)  
RN 4845-05-0 CAPLUS  
CN Hydroperoxide, 2-cyclohexen-1-yl (9CI) (CA INDEX NAME)



IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidation by, of cyclohexene, to epoxycyclohexane and epoxycyclohexanol,  
 catalysts for, selectivity of)  
 RN 7782-44-7 CAPLUS  
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

L34 ANSWER 73 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:123602 CAPLUS

DOCUMENT NUMBER: 110:123602

TITLE: Kinetic study of oxygen reduction to HO<sub>2</sub><sup>-</sup> on  
 teflon-bonded copper manganite electrodes

AUTHOR(S): Gautier, J. L.; Restovic, A.; Chartier, P.

CORPORATE SOURCE: Fac. Cienc., Univ. Santiago, Santiago, Chile

SOURCE: Boletin de la Sociedad Chilena de Quimica (1988),  
 33(4), 209-27

CODEN: BOCQAX; ISSN: 0366-1644

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

AB O<sub>2</sub> is electrocatalytically reducible in alkaline medium on Teflon-bonded  
 Cu<sub>1</sub>+xMn<sub>2</sub>-xO<sub>4</sub> electrodes showing spinel structure. The reduction is likely to  
 occur on active Mn sites through HO<sub>2</sub><sup>-</sup> formation. A mechanism for the  
 electroredn. of O<sub>2</sub> is proposed according to exptl. kinetics parameters.  
 In the region of low degrees of polarization the protonation of O<sub>2</sub><sup>-</sup> seems  
 the rate-determining step, whereas at high overpotentials the addition of the  
 first  
 electron to adsorbed O<sub>2</sub> is considered the rate-determining step. The influence  
 of the tri- and tetravalent cations in the structure on the kinetics and  
 reactions scheme is shown.

IT 12019-04-4, Copper manganese oxide (CuMn<sub>2</sub>O<sub>4</sub>) 56320-15-1,  
 Copper manganese oxide (Cu<sub>1.2</sub>Mn<sub>1.8</sub>O<sub>4</sub>) 62975-03-5, Copper  
 manganese oxide (Cu<sub>1.4</sub>Mn<sub>1.6</sub>O<sub>4</sub>) 119398-08-2, Copper manganese  
 oxide (Cu<sub>1.3</sub>Mn<sub>1.7</sub>O<sub>4</sub>) 119398-10-6, Copper manganese oxide  
 (Cu<sub>1.1</sub>Mn<sub>1.9</sub>O<sub>4</sub>)

RL: PRP (Properties)

(electrocatalyst, Teflon-bonded, for oxygen reduction in alkaline  
 solution)

RN 12019-04-4 CAPLUS

CN Copper manganese oxide (CuMn<sub>2</sub>O<sub>4</sub>) (8CI, 9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
=====	=====	=====
O	4	17778-80-2
Cu	1	7440-50-8
Mn	2	7439-96-5

RN 56320-15-1 CAPLUS

CN Copper manganese oxide (Cu<sub>1.2</sub>Mn<sub>1.8</sub>O<sub>4</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
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O	4	17778-80-2
Cu	1.2	7440-50-8
Mn	1.8	7439-96-5

RN 62975-03-5 CAPLUS

CN Copper manganese oxide (Cu<sub>1.4</sub>Mn<sub>1.604</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Cu	1.4	7440-50-8
Mn	1.6	7439-96-5

RN 119398-08-2 CAPLUS

CN Copper manganese oxide (Cu<sub>1.3</sub>Mn<sub>1.704</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Cu	1.3	7440-50-8
Mn	1.7	7439-96-5

RN 119398-10-6 CAPLUS

CN Copper manganese oxide (Cu<sub>1.1</sub>Mn<sub>1.904</sub>) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Cu	1.1	7440-50-8
Mn	1.9	7439-96-5

IT 14691-59-9P, Peroxide (HO<sub>2</sub>-)RL: FORM (Formation, nonpreparative); **PREP (Preparation)**

(formation of, in electrocatalytic reduction of oxygen on Teflon-bonded copper manganate)

RN 14691-59-9 CAPLUS

CN Peroxide (HO<sub>2</sub>-) (8CI, 9CI) (CA INDEX NAME)

-O-OH

IT 7782-44-7, Oxygen, reactions

RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**

(reduction of, copper manganate electrocatalyst bonded with Teflon for)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O



L34 ANSWER 74 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1984:174353 CAPLUS

DOCUMENT NUMBER: 100:174353

TITLE: Oxygenation of olefins under reductive conditions.  
Cobalt-catalyzed selective conversion of aromatic  
olefins to benzylic alcohols by molecular oxygen and  
tetrahydroborate

AUTHOR(S): Okamoto, Tadashi; Oka, Shinzaburo

CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Uji, 611, Japan

SOURCE: Journal of Organic Chemistry (1984), 49(9), 1589-94

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A high-yield catalytic conversion of  $\text{RC}_6\text{H}_4\text{CR}_1\text{:CHR}_2$  ( $\text{R} = \text{H}$ , 4-Cl, 2-, 4-Me, 4-MeO, 4-Br, 3-O<sub>2</sub>N;  $\text{R}_1 = \text{H}$ , Me;  $\text{R}_2 = \text{H}$ , Me, CH<sub>2</sub>OH, CH:CH<sub>2</sub>, CH<sub>2</sub>CH:CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>CH:CH<sub>2</sub>) to benzylic alcs.  $\text{RC}_6\text{H}_4\text{CR}_1(\text{OH})\text{CH}_2\text{R}_2$  (I) by mol. O<sub>2</sub> and BH<sub>4</sub>- was catalyzed by Co(TPP) (TPP = tetraphenylporphyrin). The reaction was regioselective exclusively. Comparison of the product distribution and D incorporation in the catalytic oxygenation of PhCH:CH<sub>2</sub>, the stoichiometric oxygenation of alkylcobalt complex PhCHMeCoLR<sub>3</sub>2 (II; L = pyridine, R<sub>3</sub> = dimethylglyoxime anion) and the decomposition of hydroperoxide PhCHMeOOH (III) indicated III was the primary product. III was formed by the reaction of II with mol. O<sub>2</sub>. Co(TPP) catalyzed 3 reactions in the overall catalytic process: formation of III, decomposition of III to benzylic alc. and aryl ketone, and reduction of the ketone.

IT 7782-44-7, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation by, of aromatic olefins, benzyl alcs. by, cobalt  
tetraphenylporphyrin catalyzed)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 14167-18-1 14172-90-8 23295-32-1

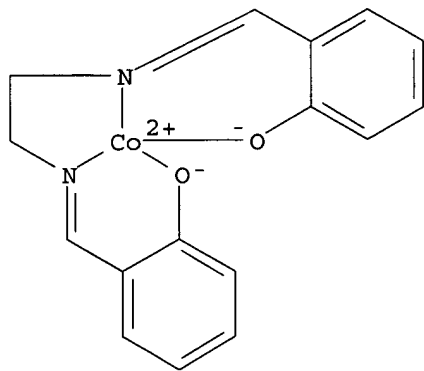
37115-10-9

RL: CAT (Catalyst use); USES (Uses)

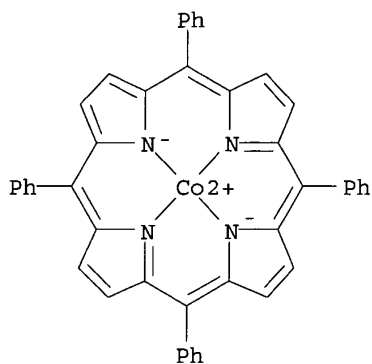
(oxidation catalyst, for aromatic olefin to benzyl alcs.)

RN 14167-18-1 CAPLUS

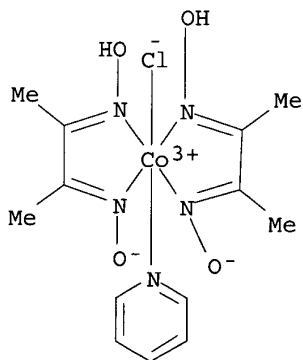
CN Cobalt, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[pheno  
lato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



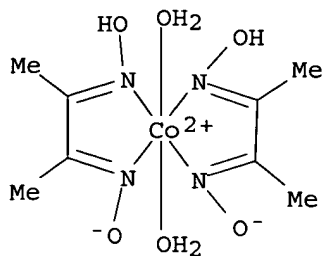
RN 14172-90-8 CAPLUS  
 CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-  
 $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]-, (SP-4-1)- (9CI) (CA INDEX  
 NAME)



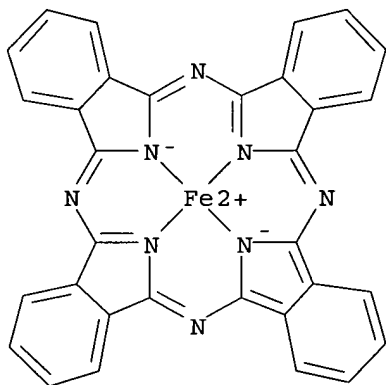
RN 23295-32-1 CAPLUS  
 CN Cobalt, bis[[2,3-butanedione di(oximato- $\kappa$ N)](1-)]chloro(pyridine)-,  
 (OC-6-42)- (9CI) (CA INDEX NAME)



RN 37115-10-9 CAPLUS  
 CN Cobalt, diaquabis[[2,3-butanedione di(oximato- $\kappa$ N)](1-)]-, (OC-6-12)-  
 (9CI) (CA INDEX NAME)



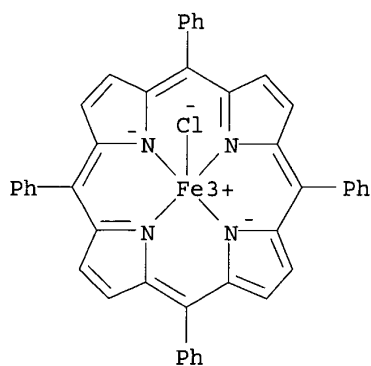
IT 132-16-1 7646-79-9, uses and miscellaneous  
 16456-81-8 19973-61-6 89556-84-3  
 RL: CAT (Catalyst use); USES (Uses)  
 (oxidation catalyst, for aromatic olefins to benzyl alcs.)  
 RN 132-16-1 CAPLUS  
 CN Iron, [29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,.kappa  
 a.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)



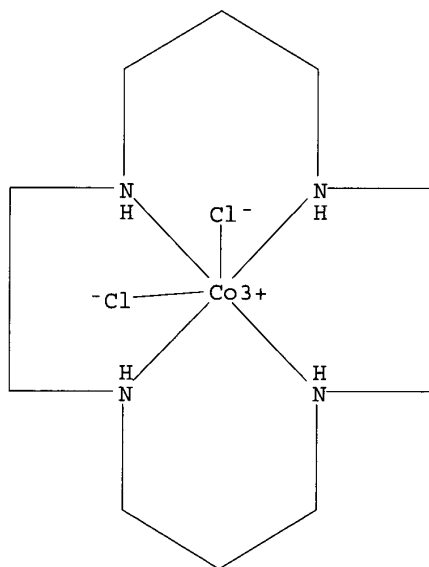
RN 7646-79-9 CAPLUS  
 CN Cobalt chloride (CoCl2) (8CI, 9CI) (CA INDEX NAME)

Cl-Co-Cl

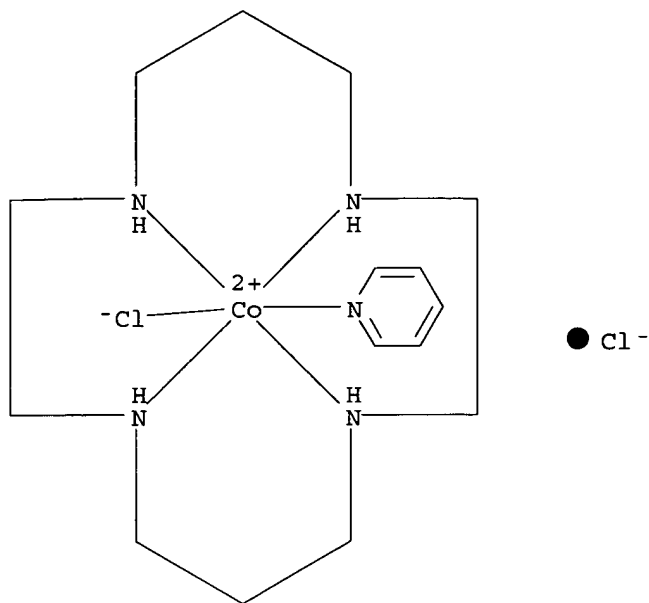
RN 16456-81-8 CAPLUS  
 CN Iron, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-  
 κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX  
 NAME)



RN 19973-61-6 CAPLUS  
 CN Cobalt(1+), dichloro(1,4,8,11-tetraazacyclotetradecane-  
 $\kappa$ N1, $\kappa$ N4, $\kappa$ N8, $\kappa$ N11)-, (OC-6-12)- (9CI) (CA INDEX  
 NAME)



RN 89556-84-3 CAPLUS  
 CN Cobalt(1+), chloro(pyridine)(1,4,8,11-tetraazacyclotetradecane-  
 N1,N4,N8,N11)-, chloride, (OC-6-23)- (9CI) (CA INDEX NAME)

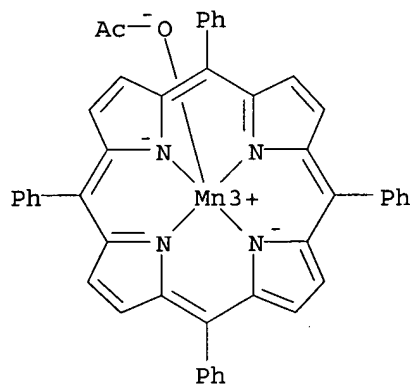


IT 58356-65-3

RL: **CAT (Catalyst use)**; **USES (Uses)**  
 (oxidation **catalyst**, for aromatic olefins, benzylic alcs. by)

RN 58356-65-3 CAPLUS

CN Manganese, (acetato- $\kappa$ O) [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)  
 )- $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]-, (SP-5-12)- (9CI) (CA  
 INDEX NAME)

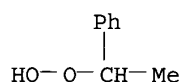


IT 3071-32-7P

RL: **RCT (Reactant)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**  
 (preparation and decomposition of)

RN 3071-32-7 CAPLUS

CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



L34 ANSWER 75 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1985:166430 CAPLUS

DOCUMENT NUMBER: 102:166430

TITLE: The liquid-phase oxidation of hydrocarbons with molecular oxygen. A selective oxidation of active cyclic methylene group to ketone group with the catalyst system composed of N,N-dialkylamides and chromium salts

AUTHOR(S): Mizukami, Fujio; Imamura, Juichi

CORPORATE SOURCE: Natl. Chem. Lab. Ind., Tsukuba, Japan

SOURCE: Kagaku Gijutsu Kenkyusho Hokoku (1984), 79(10), 515-24  
CODEN: KGKHEP; ISSN: 0388-3213

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

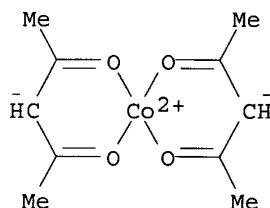
AB The metal-ion catalyzed oxidation of tetralin was carried out in solvents in which metal salts are soluble. For the production of  $\alpha$ -tetralone, a chromium salt is the best catalyst among the first-transition-metal salts and N,N-dialkylamides are the best solvents or additives. E.g., in tris(acetylacetonato)chromium(III)-catalyzed oxidation of tetralin in the presence of AcNMe<sub>2</sub>,  $\alpha$ -tetralone was obtained in 93.0% yield with 27.2% tetralin conversion.  $\alpha$ -Indanone and fluorenone are prepared in very high yields by analogous oxidation of indane and fluorene. The decomposition of  $\alpha$ -tetralinyl hydroperoxide with different first-transition-metal catalysts was also carried out in DMF in order to elucidate the formation mechanism for  $\alpha$ -tetralone in the oxidation of tetralin in the presence of N,N-dialkylamides. The product distribution in the oxidation mainly depends on the decomposition mechanism of  $\alpha$ -cyclic peroxide and that N,N-dialkylamides seem to promote the reaction of the  $\alpha$ -cyclic peroxy radical with low valent metal ions.

IT 14024-48-7

RL: CAT (Catalyst use); USES (Uses)  
(catalyst, for oxidation of tetralin with oxygen)

RN 14024-48-7 CAPLUS

CN Cobalt, bis(2,4-pentanedionato- $\kappa\text{O},\kappa\text{O}'$ )-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT 1066-30-4 1308-14-1 1333-82-0

7440-47-3D, naphthenic acid compound 7788-97-8

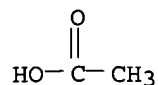
10060-12-5 10101-53-8 13548-38-4

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for liquid-phase oxidation of tetralin with oxygen)

RN 1066-30-4 CAPLUS

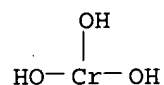
CN Acetic acid, chromium(3+) salt (8CI, 9CI) (CA INDEX NAME)



●1/3 Cr(III)

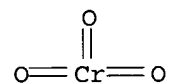
RN 1308-14-1 CAPLUS

CN Chromium hydroxide (Cr(OH)3) (8CI, 9CI) (CA INDEX NAME)



RN 1333-82-0 CAPLUS

CN Chromium oxide (CrO3) (8CI, 9CI) (CA INDEX NAME)



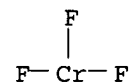
RN 7440-47-3 CAPLUS

CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

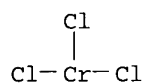
RN 7788-97-8 CAPLUS

CN Chromium fluoride (CrF3) (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 10060-12-5 CAPLUS

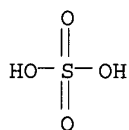
CN Chromium chloride (CrCl3), hexahydrate (8CI, 9CI) (CA INDEX NAME)



●6 H<sub>2</sub>O

RN 10101-53-8 CAPLUS

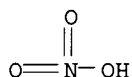
CN Sulfuric acid, chromium(3+) salt (3:2) (6CI, 8CI, 9CI) (CA INDEX NAME)



●2/3 Cr(III)

RN 13548-38-4 CAPLUS

CN Nitric acid, chromium(3+) salt (8CI, 9CI) (CA INDEX NAME)



●1/3 Cr(III)

IT 638-38-0 6018-89-9 6046-93-1 6147-53-1

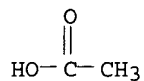
7705-08-0, uses and miscellaneous

RL: **CAT (Catalyst use)**; USES (Uses)

(**catalysts**, for oxidation of tetralin by oxygen in DMF)

RN 638-38-0 CAPLUS

CN Acetic acid, manganese(2+) salt (8CI, 9CI) (CA INDEX NAME)

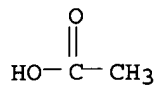


●1/2 Mn(II)

RN 6018-89-9 CAPLUS



CN Acetic acid, nickel(2+) salt, tetrahydrate (8CI, 9CI) (CA INDEX NAME)

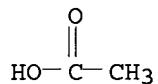


● 1/2 Ni(II)

● 2 H<sub>2</sub>O

RN 6046-93-1 CAPLUS

CN Acetic acid, copper(2+) salt, monohydrate (8CI, 9CI) (CA INDEX NAME)

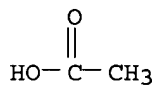


● 1/2 Cu(II)

● 1/2 H<sub>2</sub>O

RN 6147-53-1 CAPLUS

CN Acetic acid, cobalt(2+) salt, tetrahydrate (8CI, 9CI) (CA INDEX NAME)

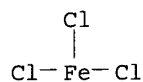


● 1/2 Co(II)

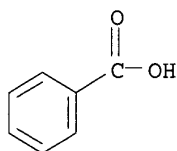
● 2 H<sub>2</sub>O

RN 7705-08-0 CAPLUS

CN Iron chloride (FeCl<sub>3</sub>) (8CI, 9CI) (CA INDEX NAME)

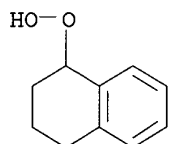


IT 932-69-4  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for oxidation of tetralin with oxygen)  
RN 932-69-4 CAPLUS  
CN Benzoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

IT 771-29-9P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, from oxidation of tetralin)  
RN 771-29-9 CAPLUS  
CN Hydroperoxide, 1,2,3,4-tetrahydro-1-naphthalenyl (9CI) (CA INDEX NAME)



IT 7782-44-7, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation by, of tetralin)  
RN 7782-44-7 CAPLUS  
CN Oxygen (8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 76 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1978:136128 CAPLUS  
DOCUMENT NUMBER: 88:136128  
TITLE: Hydrogenation of organic peroxide

INVENTOR(S): Mabuchi, Shunsuke; Tsuzuki, Kenji; Kumoi, Sadakatsu  
PATENT ASSIGNEE(S): Toyo Soda Mfg. Co., Ltd., Japan  
SOURCE: Ger. Offen., 22 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2731867	A1	19780119	DE 1977-2731867	19770714
DE 2731867	B2	19810702		
DE 2731867	C3	19820401		
JP 53009705	A2	19780128	JP 1976-83513	19760715
US 4123616	A	19781031	US 1977-806703	19770615
NL 7707883	A	19780117	NL 1977-7883	19770715
PRIORITY APPLN. INFO.:			JP 1976-83513	A 19760715

AB Aliphatic peroxides were hydrogenated in an inert solvent using a suspended Ni catalyst at a rate of 0.05-10 g/h/g catalyst at 140-200° and H pressure 10-300 kg/cm<sup>2</sup>. Thus, butadiene peroxide polymer was hydrogenated in AcOEt at 150°, 100 kg/cm<sup>2</sup> H to give 1,4-butanediol 53.5 and 1,2-butanediol 25.1%.

IT 7440-02-0, uses and miscellaneous  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for hydrogenation of aliphatic peroxides to alcs.)

RN 7440-02-0 CAPLUS

CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

IT 30946-71-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrogenation of)

RN 30946-71-5 CAPLUS

CN 1,3-Butadiene, polymer with oxygen (9CI) (CA INDEX NAME)

CM 1

CRN 7782-44-7

CMF 02

 $\text{O}=\text{O}$ 

CM 2

CRN 106-99-0

CMF C4 H6

 $\text{H}_2\text{C}=\text{CH}-\text{CH}=\text{CH}_2$

IT 4676-82-8P

RL: RCT (Reactant); **SPN (Synthetic preparation); PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and hydrogenation of)

RN 4676-82-8 CAPLUS

CN Hydroperoxide, tetrahydro-2-furanyl (9CI) (CA INDEX NAME)

